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Online-only Table 1 The list of materials and their band gaps from experiment, present work, Materials Project, OQMD, AFLOW, AFLOW (fitted), and JARVIS.

From: A band-gap database for semiconducting inorganic materials calculated with hybrid functional

Name	ICSD	Space group	Exp.	Band gap					
				Present work	Materials Project	OQMD	AFLOW	AFLOW (fitted)	JARVIS
Mg_2Pb	104846	225	0.1	0	0	0	0	0	0.32
InSb	640411	216	0.16	0.01	0	0.26	0	0	0.13
Bi_2Te_3	15753	166	0.21	0.02	0.53	0.52	0.28	1.29	-
PbTe	63098	225	0.26	0.42	0.87	0.97	0.8	1.99	1.4
$CdSnAs_2$	16737	122	0.26	0.04	0.05	0.3	0	0	-
Sb_2Te_3	193341	166	0.3	0.43	0.01	0.21	0.04	0.97	-
Cu_3SbSe_4	400652	121	0.31	0.11	0	0	0	0	-
Te	161690	152	0.33	0.69	0.41	0.5	0.15	1.12	0.62
Bi_2Se_3	617072	166	0.35	0.23	0.54	0.42	0.49	1.58	-
Mg_2Sn	104869	225	0.36	0.09	0	0	0	0	0.24
InAs	610687	216	0.36	0.1	0	0.37	0	0	0.4
PbSe	63096	225	0.37	0.36	0.47	0.69	0.4	1.45	0.96
$ZnSnSb_2$	42669	122	0.4	0.36	0	0	0	0	0.32
CoP_3	624594	204	0.43	0.11	0	0	0	0	-
CdSb	52830	61	0.46	0.52	0.14	0.19	0.09	1.03	-
Cu_3SbS_4	2857	121	0.46	0.32	0	0	0	0	-

Name	ICSD	Space group	Exp.	Band gap					
				Present work	Materials Project	OQMD	AFLOW	AFLOW (fitted)	JARVIS
PbS	62190	225	0.5	0.47	0.47	0.69	0.47	1.54	1.3
ZnSb	43265	61	0.5	0.63	0.04	0.2	0.17	1.14	-
$CuFeS_2$	60166	122	0.53	1.6	0	0	0	0	0
$CdGeAs_2$	153593	122	0.53	0.09	0.08	0.34	0.03	0.96	0.52
$CoSb_3$	153504	204	0.63	0.75	0.17	0.22	0.15	1.12	-
$ZnSnAs_2$	18203	122	0.65	0.55	0.01	0.2	0	0	0.8
Ge	41980	227	0.67	0.17	0	0	0	0	0.61
GaSb	41675	216	0.67	0.41	0	0.37	0	0	0.59
$CoAs_3$	31111	204	0.69	0.52	0	0.15	0	0	-
InN	109463	186	0.7	0.5	0	0.28	0	0	0.76
Mg_2Ge	52283	225	0.74	0.54	0.19	0.24	0.19	1.17	0.58
TlSe	44706	140	0.74	0.55	0.25	0	0.11	1.06	0.74
Mg_2Si	104864	225	0.77	0.59	0.24	0.28	0.24	1.23	0.62
$RhSb_3$	650248	204	0.8	0.16	0	0.15	0	0	-
CdO	181294	225	0.8	0.76	0	0	0	0	1.31
$CuGaTe_2$	28738	122	0.82	0.96	0.2	0.4	0.43	1.49	0.04
$RhAs_3$	34052	204	0.85	0	0	0	0	0	-
$ZnGeAs_2$	16735	122	0.85	0.84	0.05	0.34	0.17	1.14	1.07
$HgIn_2Te_4$	25652	82	0.86	1.12	0.52	0.61	0.56	1.67	1.35
$CuInSe_2$	73351	122	0.86	0.74	0.02	0.16	0	0	0.64
Cu_3AsSe_4	610361	121	0.88	0.05	0	0	0	0	-
Zn_3As_2	44091	137	0.93	0.54	0	0	0.13	1.09	-
$CuInTe_2$	169048	122	0.95	0.71	0.02	0.24	0.25	1.25	1.04
$AgInSe_2$	28751	122	0.96	0.74	0.06	0.16	0.4	1.45	1
$CuGaSe_2$	247513	122	0.96	1.08	0.04	0.25	0.4	1.45	1.39
$AgGaSe_2$	28748	122	1.1	1.24	0.25	0.41	0.7	1.86	1.56
Si	51688	227	1.12	1.19	0.62	0.77	0.61	1.74	1.28
$AgGaTe_2$	28749	122	1.15	0.9	0.19	0.32	0.52	1.62	-
Cu_2CdSnS_4	238144	121	1.16	0.97	0	0.21	0.1	1.05	-
$CdSnP_2$	22183	122	1.17	0.9	0.27	0.51	0.14	1.1	1.21
InSe	185172	194	1.17	1.18	0.46	0.55	0.43	1.5	1.43
$IrSb_3$	640958	204	1.18	0.61	0.05	0.21	0	0	0.24
$AgInS_2$	28750	122	1.18	1.26	0.38	0.49	0.92	2.16	1.62

Name	ICSD	Space group	Exp.	Band gap					
				Present work	Materials Project	OQMD	AFLOW	AFLOW (fitted)	JARVIS
$ZnIn_2Te_4$	25650	82	1.2	1.51	0.82	0.92	0.93	2.17	1.77
$CuInS_2$	66865	122	1.2	1.22	0.01	0.42	0.4	1.45	0.69
Cu_3AsS_4	14285	31	1.24	0.96	0.01	0	0.2	1.18	-
$CdIn_2Te_4$	25651	82	1.26	1.49	0.84	0.92	0.9	2.12	1.72
InP	53105	216	1.27	1.12	0.47	0.74	0.58	1.69	1.39
GaAs	41981	216	1.35	0.95	0.19	0.57	0.3	1.32	1.32
$ZnGa_2Te_4$	290911	82	1.35	1.72	1.01	1.18	1.11	2.41	1.74
CuO	16025	15	1.4	1.94	0	0	0	0	0.01
CdTe	93944	216	1.44	1.63	0.59	0.87	0.71	1.87	1.64
$HgIn_2Se_4$	25649	82	1.45	1.38	0.62	0.72	0.67	1.81	1.64
$ZnSnP_2$	22179	122	1.45	1.53	0.7	0.92	0.68	1.83	1.69
MnTe	174028	194	1.46	1.47	0	0	0	0	0
BAs	43871	216	1.5	1.86	1.21	1.42	1.2	2.53	1.93
Se (gray)	164264	152	1.5	1.76	1.06	0.88	0.98	2.23	1.71
CdTe	620518	186	1.5	1.67	0.62	0.87	0.71	1.92	1.76
$CdIn_2Se_4$	151954	82	1.55	1.77	0.95	1.03	1.04	2.31	2.16
$CdSiAs_2$	22187	122	1.6	1.14	0.4	0.69	0.46	1.53	1.33
AlSb	44325	216	1.6	1.88	1.23	1.38	1.23	2.57	1.78
$AgGaS_2$	23698	122	1.66	1.99	0.96	1.09	1.5	2.94	2.36
GaTe	635512	12	1.69	1.88	1.06	0.93	0.89	2.12	1.72
$ZnSiAs_2$	22184	122	1.7	1.67	0.89	1.06	1.12	2.42	1.85
CdSe	41826	186	1.74	1.47	0.57	0.77	0.69	1.84	2.06
$CdGeP_2$	100467	122	1.8	1.33	0.64	0.9	0.7	1.85	1.65
$ZnIn_2Se_4$	25647	82	1.82	1.83	0.98	1.12	1.13	2.44	2.22
$HgGa_2Se_4$	188545	82	1.95	1.72	0.91	1.05	0.95	2.2	2.08
GaSe	63122	194	2.02	1.77	1.23	0.97	0.81	2.01	2.14
$CuAlTe_2$	28735	122	2.06	1.88	1.02	1.2	1.29	2.65	1.82
BP	615154	216	2.1	1.97	1.24	1.37	1.25	2.59	1.91
AlAs	185081	216	2.16	2.15	1.52	1.63	1.5	2.94	2.28
$ZnGeP_2$	16734	122	2.2	1.83	1.19	1.37	1.25	2.59	1.93
$CdSiP_2$	22188	122	2.2	1.99	1.43	1.4	1.41	2.81	2.02
$ZnGa_2Se_4$	44887	82	2.2	2.34	1.39	1.54	1.55	3	2.84
AgI	164963	216	2.22	2.49	1.37	1.48	1.98	3.58	2.87
GaP	77087	216	2.24	2.43	1.59	1.75	1.64	3.13	2.37

Name	ICSD	Space group	Exp.	Band gap					
				Present work	Materials Project	OQMD	AFLOW	AFLOW (fitted)	JARVIS
ZnTe	185141	216	2.26	2.19	1.08	1.45	1.48	2.9	2.23
$ZnSiP_2$	22190	122	2.3	1.92	1.36	1.44	1.38	2.77	2.03
β-SiC	603798	216	2.3	2.26	1.39	1.59	1.37	2.76	2.31
$AgAlTe_2$	28746	122	2.35	1.84	1.05	1.2	1.36	2.75	1.99
CdS	154186	186	2.42	2.38	1.12	0.77	1.25	2.6	2.6
$CdGa_2Se_4$	2287	82	2.43	2.22	1.35	1.45	1.41	2.82	2.72
AlP	24490	216	2.45	2.33	1.63	1.75	1.63	3.11	2.56
$AgAlSe_2$	28745	122	2.5	2.17	1.14	1.33	1.56	3.02	2.36
ZnSe	185134	216	2.58	2.54	1.17	1.5	1.7	3.2	2.63
La_2S_3	15151	62	2.73	1.75	1.03	1.2	0.92	2.16	-
AgI	62789	186	2.63	2.52	1.4	1.55	1.98	3.61	2.85
$CuAlSe_2$	28734	122	2.65	2.08	0.9	1.07	1.24	2.58	2.51
BeTe	53945	216	2.8	2.69	2.02	2.15	2.02	3.63	2.82
$HgGa_2S_4$	189737	82	2.84	2.57	1.57	0.72	1.62	3.1	2.83
α-SiC	164429	186	2.86	2.94	2.04	2.15	2.02	3.63	3.08
CuBr	23989	216	2.91	2.12	0.49	0.62	1.13	2.44	1.55
CuI	33724	216	2.95	2.56	1.14	1.29	1.65	3.14	2.2
Al_2Se_3	14373	9	3.1	2.77	1.81	1.86	1.76	3.28	2.85
CuCl	23988	216	3.17	2.33	0.56	0.64	1.28	2.64	1.58
CeO_2	184584	225	3.2	3.36	1.87	2.1	2.42	4.17	2.01
ZnO	154486	186	3.2	2.66	0.73	1.04	1.82	3.37	2.47
GaN	153890	186	3.34	2.94	1.74	2.09	1.91	3.49	3.08
$CuAlS_2$	189083	122	3.35	3.04	1.69	1.88	2.05	3.67	2.49
FeF_2	14143	136	3.4	3.63	3.38	0.42	2.63	4.46	0
$ZnGa_2S_4$	44886	82	3.4	3.31	2.27	2.41	2.44	4.2	3.86
$CdGa_2S_4$	106362	82	3.44	3.12	2.12	1.45	2.21	3.89	3.71
SnO_2	154960	136	3.47	2.29	0.65	1.2	0	0	2.39
ZnS	77090	216	3.54	3.61	2.02	2.32	2.68	4.52	3.59
BeSe	616419	216	3.61	3.54	2.69	2.82	2.67	4.51	3.88
MnO	9864	225	3.9	2.85	1.72	0.42	2.62	4.44	0
SrS	651054	225	4.1	3.46	2.5	2.59	2.5	4.28	3.61
BeS	44724	216	4.17	4.1	3.15	3.23	3.14	5.15	4.38
NiO	43740	225	4.5	4.53	2.31	2.62	2.22	3.91	0.01
RMSE				0.36	1.05	1.02	0.93	0.75	0.85

1. The experimental data were adopted from a CRC Handbook[39] except $AgAlSe_2$[40], $AgAlTe_2$[40], $AgGaTe_2$[40], CdO_2[41], $CdSnP_2$[42], $CuAlS_2$[43], $CuAlTe_2$[44], $HgIn_2Se_4$[45], and InN[46] for which more reliable measurements are cited, and CeO_2[47] and La_2S_3[48] which represent lanthanides.

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