supplemental materials: Laplacian free and asymptotic corrected semilocal exchange potential applied to band gap of solids

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In this supplemental material for the article "Laplacian free and asymptotic corrected semilocal exchange potential applied to the band gap of solids", first, we present band gaps of a set of well known solids in Table 1, using the potentials discussed in the article. The band gaps for PBE functional underestimates in all cases. In addition to PBE, we show band gaps for TBMBJ, mBR-TBMBJ, HSE methods and compared to the experimental values. It can be observed that the mean absolute errors (MAE) for mBR-TBMBJ and HSE are same and better than TBMBJ. Fig. 1 represents the box plot for the absolute errors of all the methods present in Table 1. Then the space groups of all the oxides, dichalcogenides, and oligoacenes are given in TABLE 2 and TABLE 3. A 3×3 supercell of silicon doped graphenes of different percentage of concentrations are shown.

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Table 1: Fundamental band gaps of semiconducting well known solids.

Solids	PBE	TBMBJ	mBR-TbmBJ	HSE06	Expt.
AgCl	0.90	2.82	3.11	2.41	3.25
AgBr	0.66	2.34	2.60	2.01	2.71
AlP	1.58	2.29	2.59	2.30	2.50
AlAs	1.44	2.12	2.64	2.11	2.23
AlSb	1.23	1.78	1.91	1.80	1.69
AgI	1.33	2.68	2.98	2.48	2.91
Al_2O_3	6.34	8.52	8.69	8.08	8.80
BaS	2.25	3.32	3.72	3.11	3.88
BaSe	1.98	2.87	3.22	2.79	3.58
BaTe	1.59	2.27	2.55	2.31	3.08
BAs	1.18	1.67	1.82	1.86	1.46
BeO	7.68	10.17	10.31	9.48	10.6
BP	1.27	1.92	2.08	1.98	2.10
CaO	3.67	5.34	5.55	5.26	7.00
CaF_2	7.32	10.52	10.88	9.37	11.8
CdTe	0.75	1.76	1.99	1.57	1.61
CuCl	0.48	1.64	1.62	2.37	3.4
CuBr	0.37	1.57	1.58	2.15	3.07
CuI	1.12	2.15	2.18	2.65	3.12
Cu_2O	0.62	0.93	0.94	1.98	2.17
CuSCN	2.25	2.66	2.67	3.60	3.94
GaP	1.63	2.3	2.57	2.28	2.35
GaSb	0.11	1.00	1.02	0.88	0.82
InP	0.66	1.62	1.83	1.43	1.42
InAs	0.00	0.74	0.90	0.45	0.42
InSb	0.00	0.48	0.59	0.45	0.24
InN	0.02	0.94	0.83	0.70	0.72
MgTe	2.49	4.11	4.52	3.39	3.60
SiO_2	5.84	7.70	7.68	7.39	8.90
SnO_2	1.57	3.43	3.42	2.88	3.60
SnTe	0.06	0.18	0.32	0.17	0.36
Sb_2Te_3	0.16	0.30	0.30	0.31	0.28
SnSe	0.58	0.78	0.96	0.98	0.90
$SrTiO_3$	1.92	2.72	2.79	3.29	3.30
TiO_2	2.14	2.99	3.07	3.57	3.40
VO_2	0.00	0.54	0.55	1.03	0.60
ZnO	0.75	2.65	2.42	3.30	3.44
MAE	1.49	0.53	0.49	0.49	–

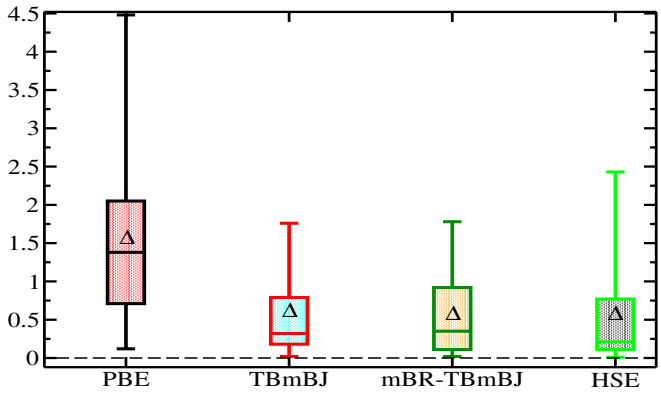

Figure 1: Box plot for the mean absolute error of semiconducting solids present in Table 1. The explanations about the box plot can be found in the main article.

Table 2: Space groups of discussed oxides, and Transition metal dichalcogenides used in the article.

Oxides	Space groups	TMDs	Space groups
BiCuOS	129(P4/nmm)	HfS_2	164(P-3m1)
BiCuOTe	129(P4/nmm)	$HfSe_2$	164(P-3m1)
LaCuOS	129(P4/nmm)	MoS_2	194(P63/mmc)
LaCuOTe	129(P4/nmm)	$MoSe_2$	194(P63/mmc)
Ag_2PdO_2	71(Imm)	WS_2	194(P63/mmc)
$CuAlO_2$	166(R-3m)	WSe_2	194(P63/mmc)
$LiCoO_2$	166(R-3m)	ZrS_2	164(P-3m1)
$BaSnO_3$	221(Pm-3m)	$ZrSe_2$	164(P-3m1)
$NaBiO_3$	148(R-3)	ZrSeS	156(P3m1)
$LiBiO_3$	56(Pccn)		
$LaMnO_3$	62(Pnma)		
$PbTiO_3$	99(P4mm)		
$BaTiO_3$	221(Pm-3m)		
$LiNbO_3$	161(R3c)		

Table 3: Space groups of discussed Transition metal monoxides and oligoacenes used in the article.

TMOs	Space groups	Oligoacenes	Space groups
CoO	166(R-3m)	Napthalene(2A)	14(P21/c)
FeO	166(R-3m)	Anthracene(3A)	14(P21/n)
MnO	166(R-3m)	Tetracene(4A)	2(P-1)
NiO	166(R-3m)	Pentacene(5A)	2(P-1)

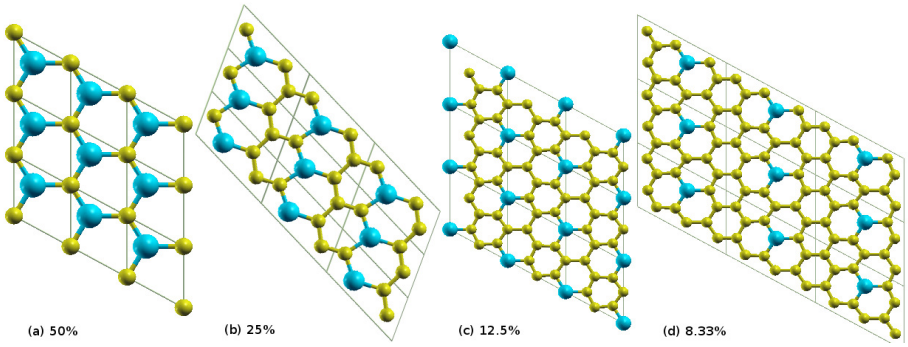

Figure 2: 3×3 supercells of different percentage silicon doped graphene sheets are shown. Golden color balls represent carbon and cyan represens silicon.