supplemental materials:Accurate band gaps from exchange potentials designed from cuspless hydrogen exchange hole model

Abhilash Patra,[1, a)] Bikash Patra,[1] and Prasanjit Samal[1, b)]
School of Physical Sciences, National Institute of Science Education and Research, HBNI, Bhubaneswar 752050, India

In this supplemental material, We collect GLLB-SC band gaps that have been used to calculate the mean absolute errors for the comparison purpose. Table S1 presents PBE band gaps of Transition metal dichalcogenides as calculated from WIEN2k code and band gaps of GLLB-SC potentials. Also, we collect the quasiparticle gaps from other literature. We mention that the collected band gaps might be obtained with different lattice parameters than our unit cell. Similarly, the band gaps of wide bandgap solids are presented in Table S2. In Fig. S1, the PBE band structure of two three-dimensional topological insulators Bi_2Se_3 and Bi_2Te_3 is presented.

TABLE S1. Band Gaps of thransition metal dichalcogenides as obtained from PBE exchange correlation energy functional and GLLB-SC potential. The GW band gaps are collected from available literatures.

Materials	Expt.	PBE	GLLB-SC	GW
ReS_2	1.37	1.21	1.80	1.57[1]
$ReSe_2$	1.19	1.05	1.60	1.38[2]
RuS_2	1.45	0.92	1.85	
$RuSe_2$	0.76	0.56	1.24	
$RuTe_2$	0.49	0.19	0.60	
HfS_2	1.96	0.93	1.99	1.96[3]
$HfSe_2$	1.13	0.48	1.17	1.26[3]
MoS_2	1.23	0.89	1.41	1.23[4]
$MoSe_2$	1.09	0.82	1.31	1.11[4]
$MoTe_2$	1.03	0.74	1.17	
WS_2	1.35	0.99	1.52	1.30[4]
Wse_2	1.20	0.95	1.50	1.19[4]
ZrS_2	1.68	0.80	1.87	1.80[3]
$ZrSe_2$	1.18	0.36	1.14	1.12[3]
MAE	–	0.44	0.22	

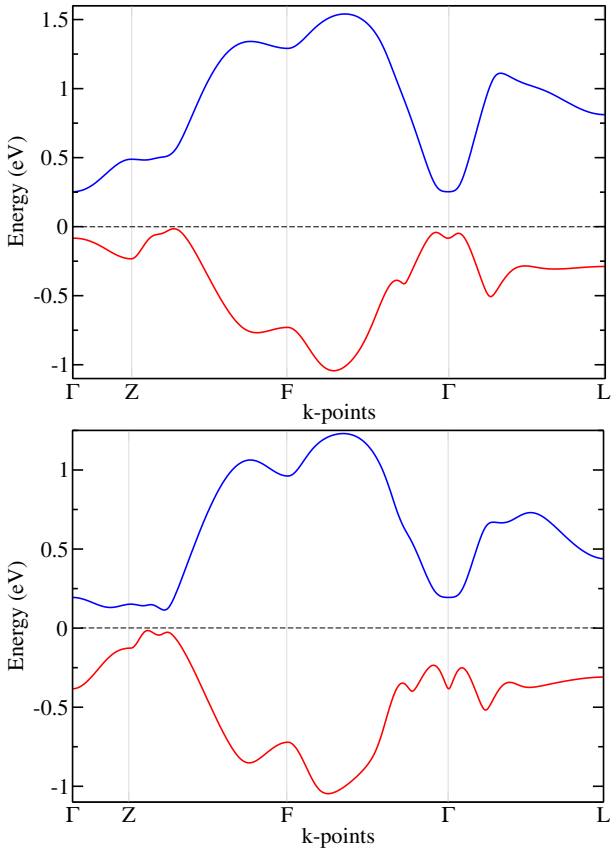

FIG. S1. Band structure of Bi_2Se_3 (left) and Bi_2Te_3 (right) as obtained by using PBE XC functional. The pronounced 'm' like behavior is clear at the Γ point in both the cases.

REFERENCES

[1]M. Gehlmann, I. Aguilera, G. Bihlmayer, S. Nemšák, P. Nagler, P. Gospodarič, G. Zamborlini, M. Eschbach, V. Feyer, F. Kronast, E. Młyńczak, T. Korn, L. Plucinski, C. Schüller, S. Blügel, and C. M. Schneider, Nano Letters **17**, 5187 (2017), pMID: 28759250.
[2]J. P. Echeverry and I. C. Gerber, Phys. Rev. B **97**, 075123 (2018).
[3]H. Jiang, The Journal of Chemical Physics **134**, 204705 (2011), https://doi.org/10.1063/1.3594205.
[4]H. Jiang, The Journal of Physical Chemistry C **116**, 7664 (2012), https://doi.org/10.1021/jp300079d.
[5]I. H. Nwigboji, J. I. Ejembi, Y. Malozovsky, B. Khamala, L. Franklin, G. Zhao, C. E. Ekuma, and D. Bagayoko, Materials Chemistry and Physics **157**, 80 (2015).
[6]M. Kolos and F. Karlicky, Phys. Chem. Chem. Phys. **21**, 3999 (2019).
[7]M. Shishkin, M. Marsman, and G. Kresse, Phys. Rev. Lett. **99**, 246403 (2007).
[8]J. M. Crowley, J. Tahir-Kheli, and W. A. Goddard, The Journal of Physical Chemistry Letters **7**, 1198 (2016), pMID: 26944092.
[9]J.-M. Mewes, P. Jerabek, O. R. Smits, and P. Schwerdtfeger, Angewandte Chemie (International ed. in English) **58**, 14260 (2019), 31343819[pmid].

[a)]Electronic mail: abhilashpatra@niser.ac.in
[b)]Electronic mail: psamal@niser.ac.in

TABLE S2. Band Gaps of twenty seven wide gap solids as obtained from PBE exchange correlation energy functional and GLLB-SC potential.

Materials	Expt.	PBE	GLLB-SC	
AlN	6.11	4.14	6.52	6.28[5]
BN	6.36	4.46	6.69	6.1[6]
BaO	4.80	2.07	4.7	
MgO	7.67	4.72	8.23	9.16[7]
CaO	6.88	3.75	7.33	6.61[a]
BeO	10.59	7.37	10.99	11.59[a]
CaS	4.43	2.38	4.72	
BeSe	5.5	2.63	4.26	
CaH_2	4.4	2.98	5.82	
$PbCl_2$	4.86	3.88	6.32	
$CaCl_2$	6.9	5.56	9.87	
NaI	5.8	3.64	6.76	6.24[a]
LiH	4.94	3.68	6.49	
LiF	13.6	9.00	14.95	15.9[7]
LiCl	9.4	6.36	10.43	8.75-10.98[8]
LiBr	7.6	4.88	8.34	
KCl	8.69	5.23	9.89	8.48[a]
KBr	7.80	4.36	8.46	
NaCl	8.75	5.08	9.48	8.75[a]
NaBr	7.1	4.12	7.86	
RbF	10.4	5.78	11.37	
RbCl	8.3	5.07	9.76	
RbBr	7.2	4.35	8.47	
SiO_2	8.9	6.01	9.98	8.77[a]
Ar	14.15	8.68	15.00	14.9[7]
Kr	11.59	7.26	12.39	11.64[9]
Xe	9.29	6.22	10.25	9.29[9]
MAE	–	2.90	0.96	–

a-G_0W_0 gaps from Ref.[10],

[10] A. Morales-García, R. Valero, and F. Illas, The Journal of Physical Chemistry C **121**, 18862 (2017).