Supplementary Material (ESI)

First-principles study on the electronic and optical properties of Bi_2WO_6

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	Lattice constants (Å)			Volume ($Å^3$)
	a	b	c	V_0
Bi_2WO_6 - exp	5.4372	16.4302	5.4584	487.21
Bi_2WO_6 - PBE	5.5532	16.8018	5.5899	521.56
Bi_2WO_6 - PBE + SOC	5.56207	16.8863	5.61217	527.1108

Table S1. The lattice constants (Å) and equilibrium volume ($Å^3$) of Bi_2WO_6. The optimized parameters from PBE and without SOC were selected for further calculations as they are closer to the experimental values.

Bi_2WO_6	Band gap E_g (eV)	Nature of the gap
Exp.[1]	2.80	Indirect
PBE	2.32	Direct
PBE + U	2.71	Direct
PBE + SOC	2.26	Indirect
PBE + U + SOC	2.61	Indirect

Table S2. Band gap comparison of Bi_2WO_6. All these calculations were performed using PesudoDojo potentials.

Element	Type	Pseudopotential file name	Source	Link
Bi	Both, with and without SOC including Non-Linear Core Correction (NLCC) Valance: $5d^{10}6s^26p^3$	Bi.upf	PesudoDojo	1
	Without SOC and without NLCC Valance: $5d^{10}6s^26p^3$	Bi_ONCV_PBE-1.2.upf	SG15 ONCV	2
	Without SOC, without NLCC and including Bi 5s and 5p as valance Valance: $5s^25p^6\,5d^{10}6s^26p^3$	Bi_oncvpsp_sr.upf	Generated using ONCVPSP code	3
	With SOC, without NLCC and including Bi semi-core (5s and 5p) as valance Valance: $5s^25p^6\,5d^{10}6s^26p^3$	Bi_oncvpsp_fr.upf	Generated using ONCVPSP code	4
W	With and without SOC including Non-Linear Core Correction (NLCC) Valance: $5d^46s^2$	W.upf	PesudoDojo	1
	Without SOC, without NLCC (including one W semi-core state, 4f as valance) Valance: $4f^{14}5d^46s^2$	W_ONCV_PBE-1.2.upf	SG15 ONCV	2
	With SOC, without NLCC (including one W semi-core state, 4f as valance) Valance: $4f^{14}5d^46s^2$	W_ONCV_PBE_FR-1.0.upf	SG15 ONCV	2
O	With and without SOC including Non-Linear Core Correction (NLCC) Valance: $2s^22p^4$	O.upf	PesudoDojo	1
	Without SOC and without NLCC Valance: $2s^22p^4$	O_ONCV_PBE-1.2.upf	SG15 ONCV	2
	With SOC, without NLCC Valance: $2s^22p^4$	O_ONCV_PBE_FR-1.0.upf	SG15 ONCV	2

Table S3. List of different pseudopotentials used in this work. The SG15 ONCV and the Bi generated ONCV PP were used in GW and followed by BSE calculations. The rest of the calculations were performed using PesudoDojo potentials. The valance electronic configurations of all the elements involved is also mentioned.

1. http://www.pseudo-dojo.org/index.html
2. http://www.quantum-simulation.org/potentials/sg15_oncv/
3. https://github.com/haseebphysics1/DFT/blob/main/Bi2WO6/PP/Bi_oncvpsp_sr.upf
4. https://github.com/haseebphysics1/DFT/blob/main/Bi2WO6/PP/Bi_oncvpsp_fr.upf

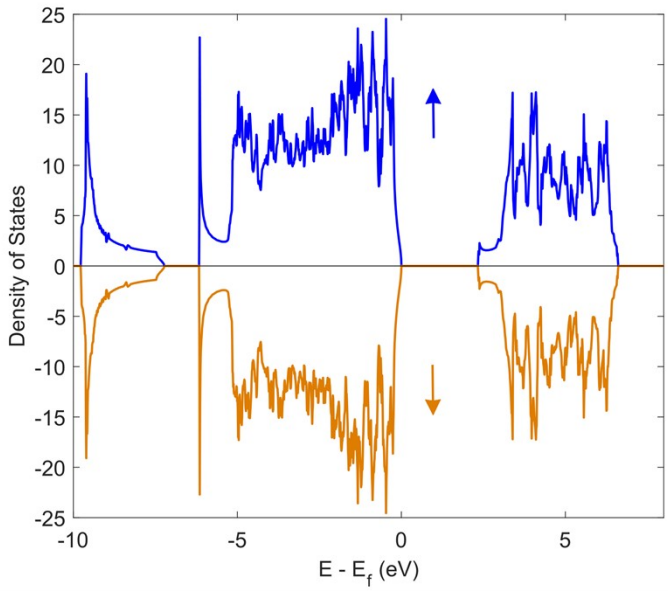

Fig S1. The DOS of Bi_2WO_6, Spin-up (blue) and spin-down (brown). The complete identical DOS confirms that we can avoid spin-polarized (magnetic) calculations.

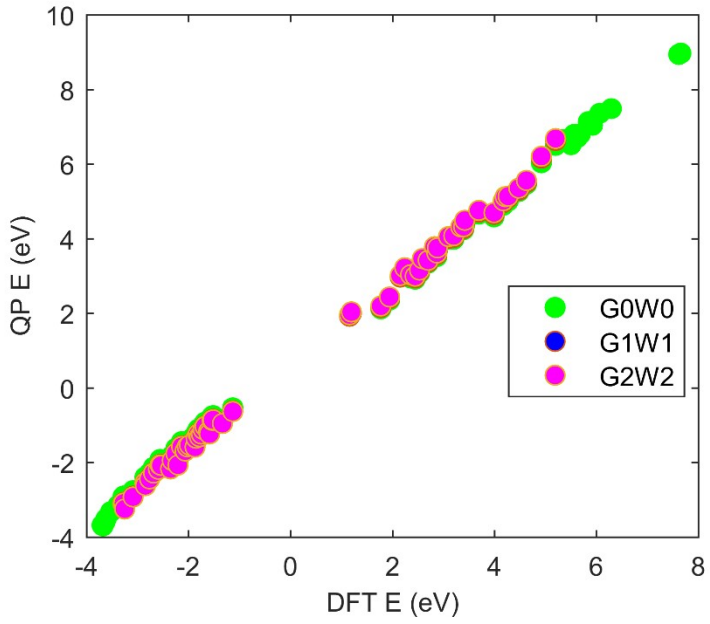

Fig S2. QP energies vs DFT: QP energies shown are computed at ^{G_0W_0}, ^{G_1W_1}, ^{G_2W_2} levels, while ^{G_3W_3} is not shown being identical to ^{G_2W_2}. The results are for selected bands around Fermi level at a single k-point to check the convergence.

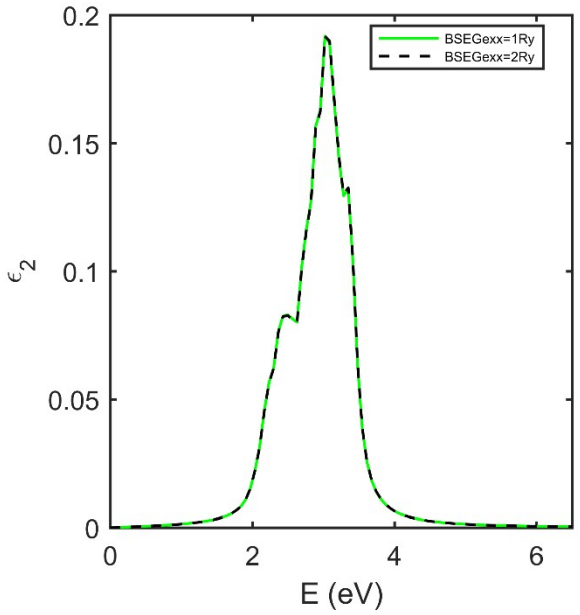

Fig S3. "BSEGexx" named parameter here defines the number of G-vectors to be summed in the exchange part of the BSE kernel. The value of 2 Ry was selected in all further calculations.

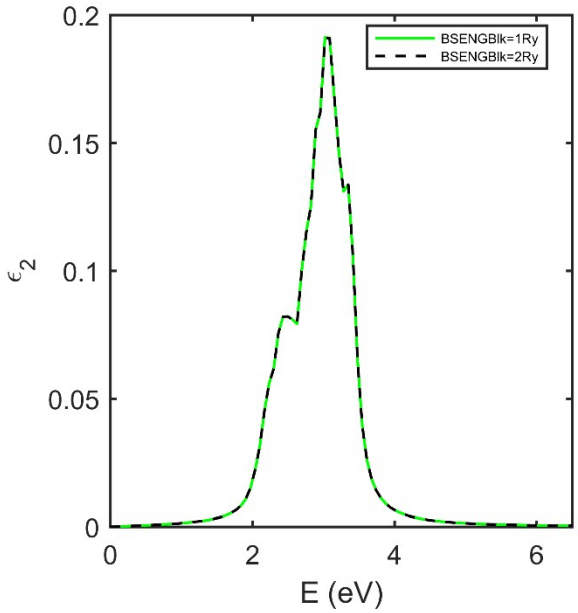

Fig S4. The number of reciprocal lattice vector components used in the Screened Coulomb Potential matrix to build the electron-hole attractive kernel. 1 Ry value was selected for further calculation for this parameter.

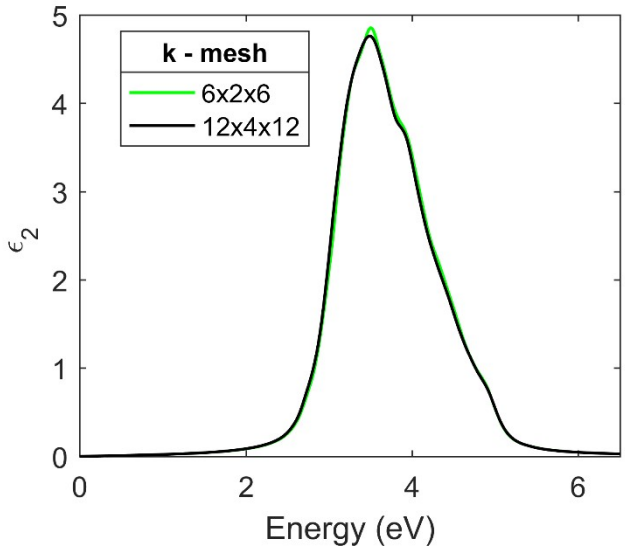

Fig S5. The imaginary part of the dielectric function from BSE calculations (with SOC). Both the calculations were performed under same numerical parameters apart from the number of k-points.

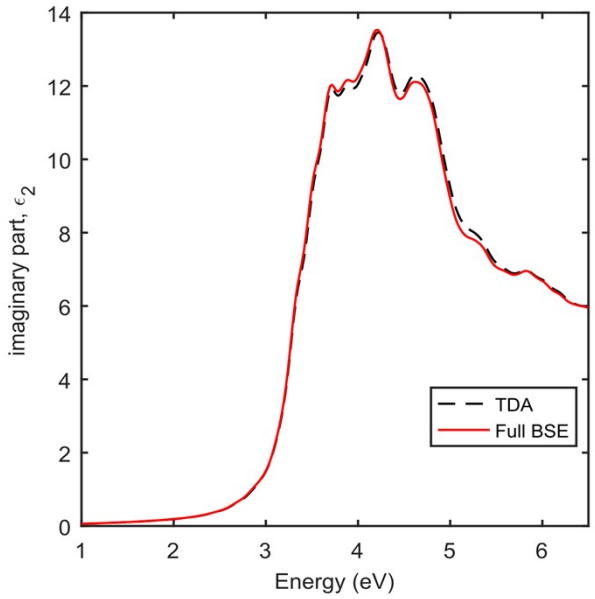

Fig S6. The comparison between TDA vs BSE with coupling between electron-hole. Two curves are almost identical which means TDA works perfectly fine for Bi_2WO_6.

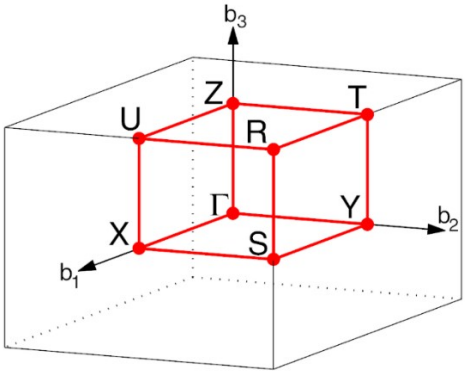

Fig S7. K-path of the Brillion zone for the orthorhombic unit cell.

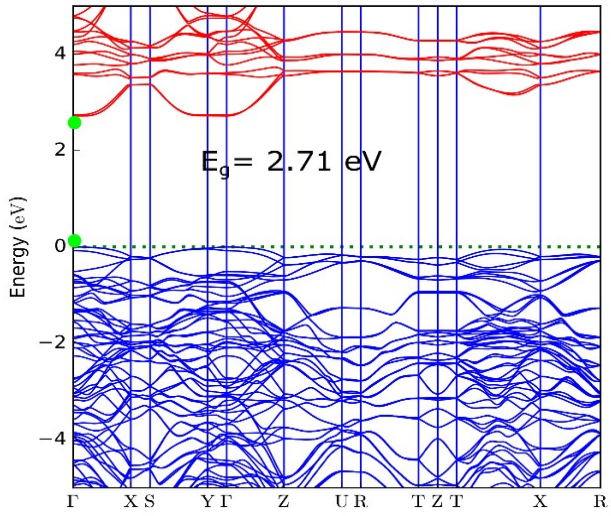

Fig S8. Band structure of Bi_2WO_6 without SOC with Hubbard parameters.

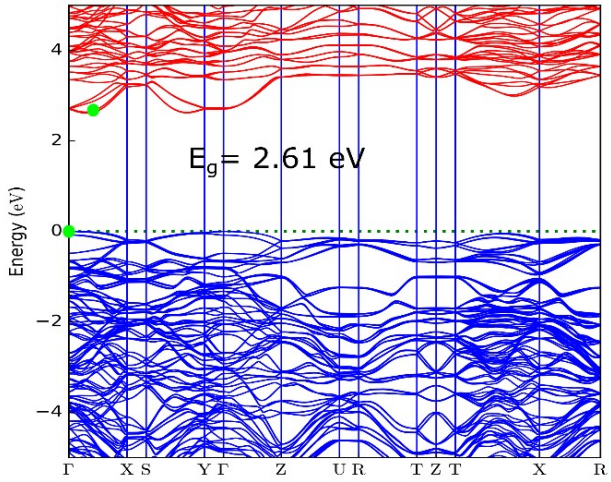

Fig S9. Band structure of Bi_2WO_6 with SOC with Hubbard parameters.

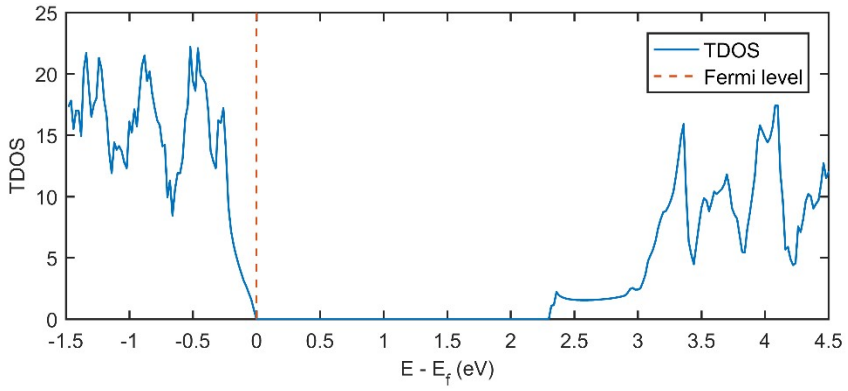

Figure S10. Total density of states of Bi2WO6 without SOC at PBE level using PseudoDojo potentials. Band gap correction was not taken into account in these results.

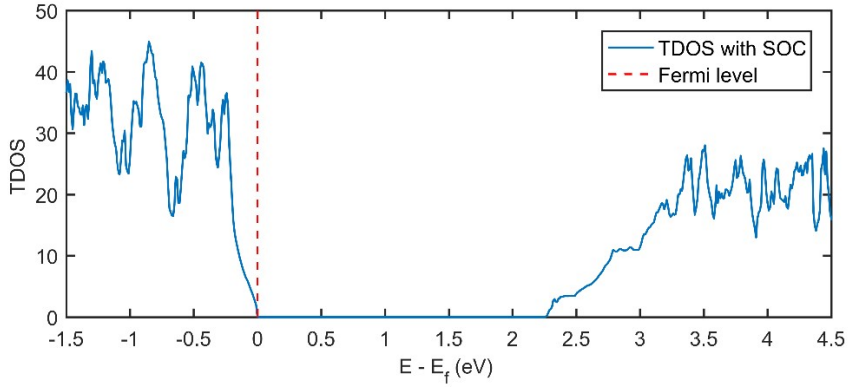

Figure S11. Total density of states of Bi2WO6 with SOC at PBE level using PseudoDojo potentials. Band gap correction was not taken into account in these results.