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Supplementary material for

Two Dimensional β-InSe with Layer-Dependent Properties: Band Alignment, Work Function and Optical Properties

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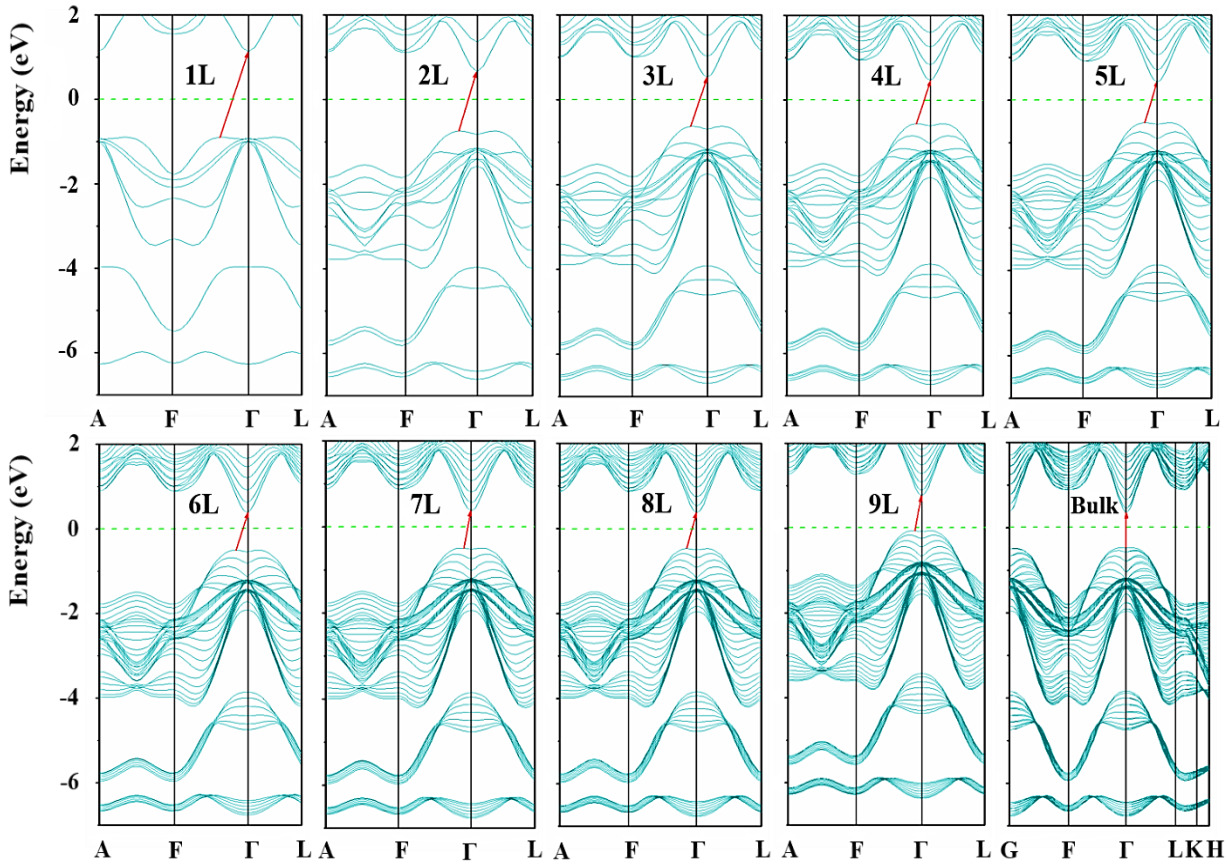

Figure S1: Electronic band structures of β-InSe monolayer (1L), few-layer (2L to 9L) and bulk β-InSe extracted from GGA-PBE functional calculations. The green dashed line is Fermi energy level set to 0.0 eV.

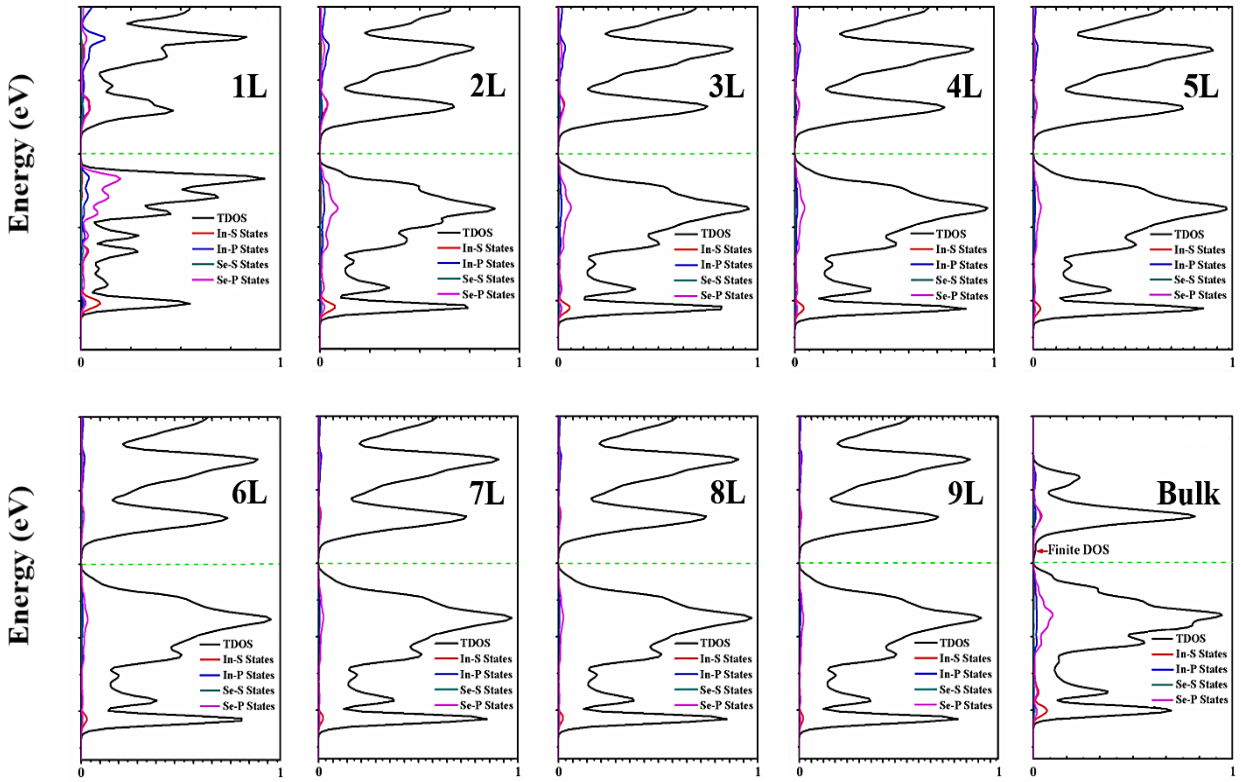

Figure S2: Calculated total density of states (TDOS) and partial density of states (PDOS) of β-InSe monolayer (1L), and few layer (2L to 9L) and bulk β-InSe based on GGA-PBE functional. The green dashed line is Fermi energy level set to 0.0 eV.

Table S1: Tabulation of band gap energy values extracted from different functional calculations of β-InSe monolayer (1L), few-layer (3L and 5L) and bulk β-InSe.

Number of layer (L)	GG-PBE (eV)	optB86b-vdW (eV)	optPBE-vdW (eV)	HSE06 (eV)
1	2.02	1.97	1.98	2.84
3	1.16	1.05	1.84	1.98
5	0.950	0.894	0.987	1.84
Bulk β-InSe	0.674	0.685	0.705	1.39

Table S2: Tabulation of band gap energy values extracted from DFT calculations of β-InSe monolayer (1L), few-layer (2L to 9L) and bulk β-InSe based on GGA-PBE.

Number of layer (L)	Band gap values (eV)	Number of layer (L)	Band gap values (eV)
1	2.02	6	0.897
2	1.40	7	0.861
3	1.16	8	0.840
4	1.03	9	0.817
5	0.950	Bulk β-InSe	0.674

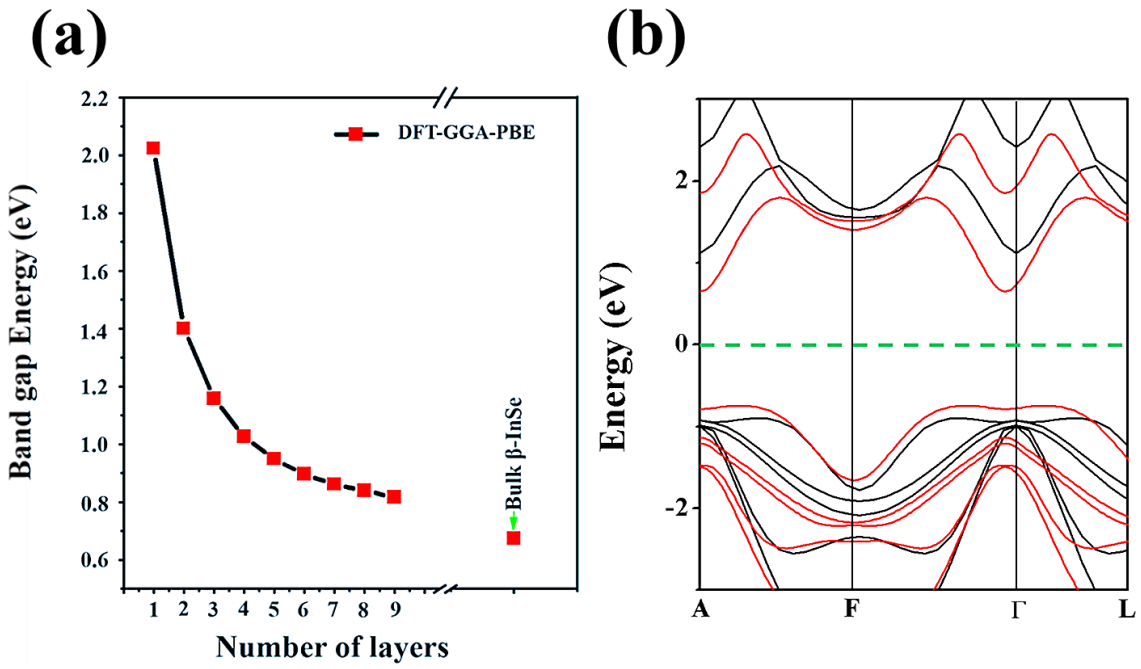

Figure S3: (a) GGA-PBE band gap energies of few-layer of β-InSe as a function of number of layer, (b) electronic band structure of monolayer β-InSe extracted from GGA-PBE calculations, band dispersion line with red is for band with SOC (E_g = 1.40 eV) and with black is for band without SOC (E_g = 1.42 eV). The green dashed line is Fermi energy level set to 0.0 eV.

Table S3: Tabulation of work function values of β-InSe monolayer (1L), few-layer (2L to 9L) and bulk β-InSe.

Number of layer (L)	Work function (eV)	Number of layer (L)	Work function (eV)
1	5.22	6	5.00
2	5.05	7	4.99
3	5.02	8	4.99
4	5.01	9	4.98
5	5.00	Bulk β-InSe	4.77

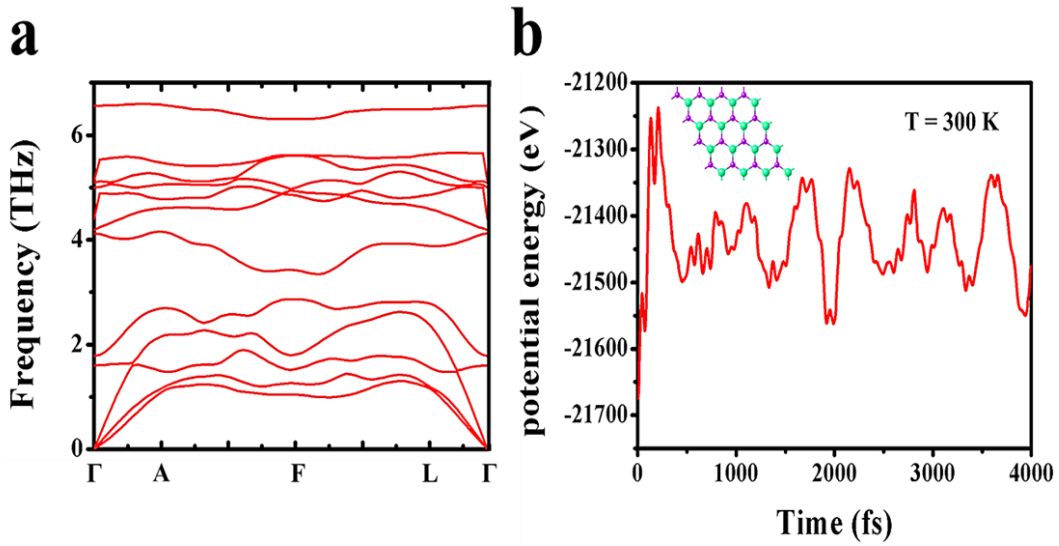

Figure S4: (**a**) Calculated phonon band dispersion structure of β-InSe a long high-symmetry direction Γ-Z-M-A-Γ (**b**) Total potential energy fluctuation of β-InSe monolayer from 500 to 4000 fs during AIMD simulations at the temperature of 300K.The inset show the snapshot at 1 ps

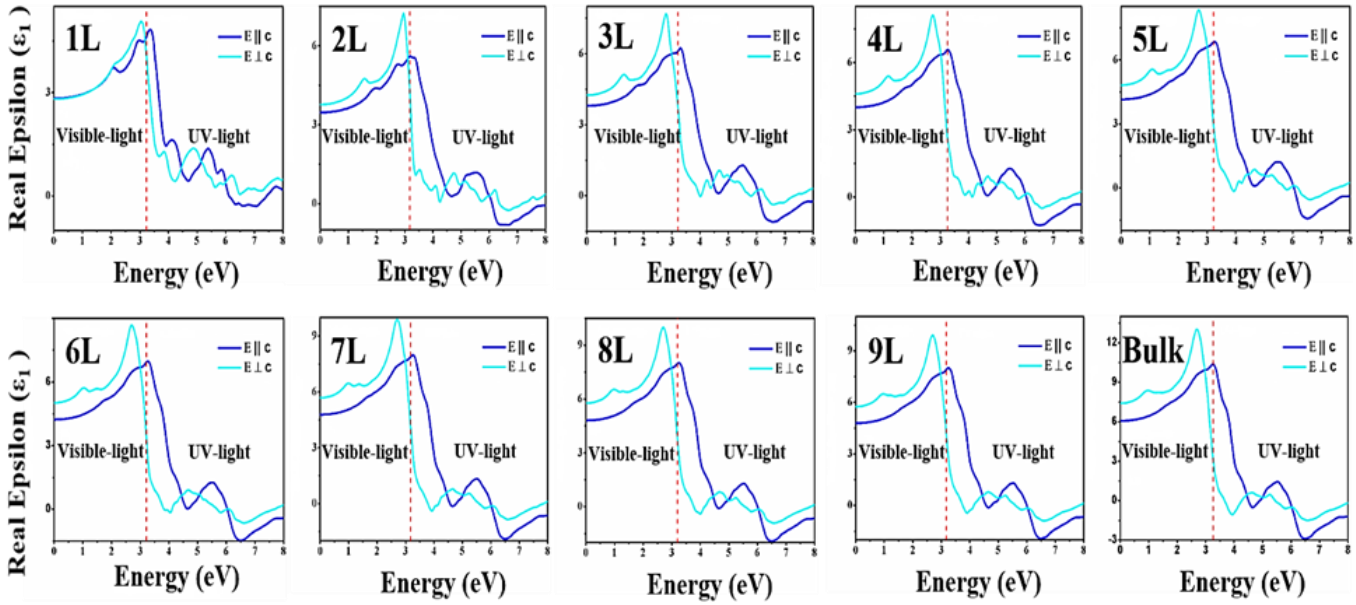

Figure S5: Calculated real part of the dielectric function along x and z direction for β-InSe monolayer (1L), few-layer (2L to 9L) and bulk β-InSe.

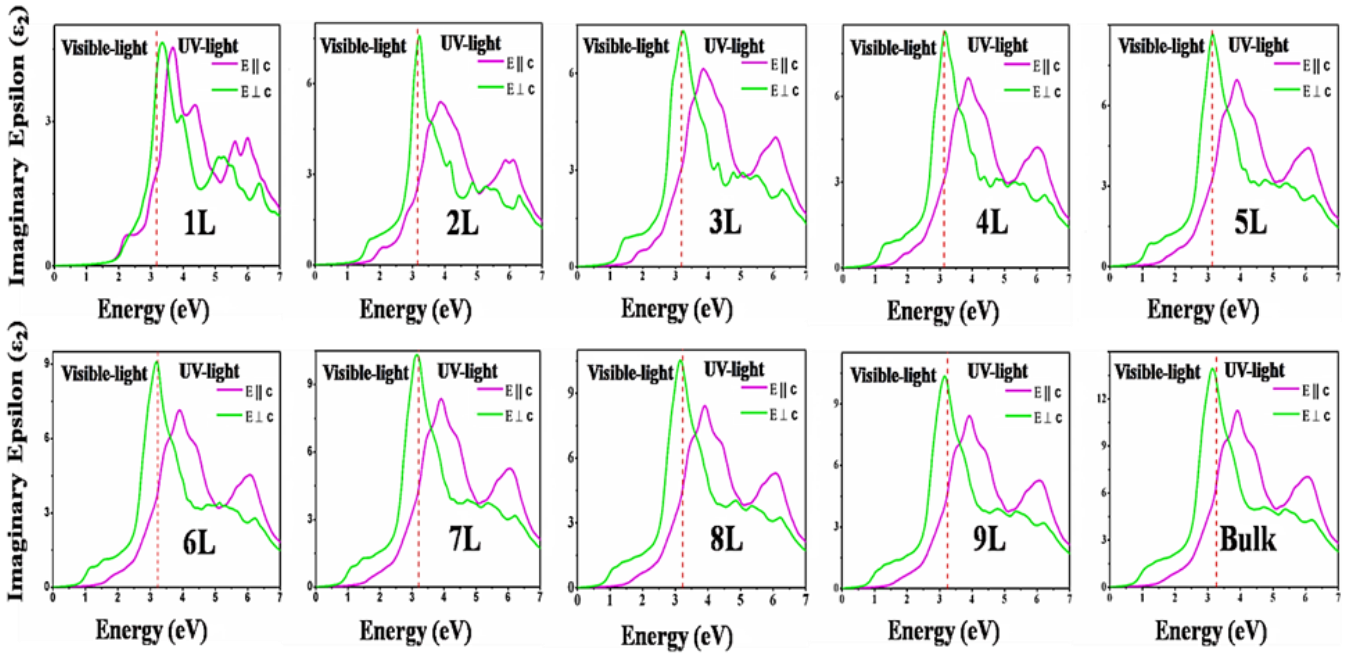

Figure S6: Calculated imaginary part of the dielectric function along x and z directions for β-InSe monolayer (1L), few-layer (2L to 9L) and bulk β-InSe.

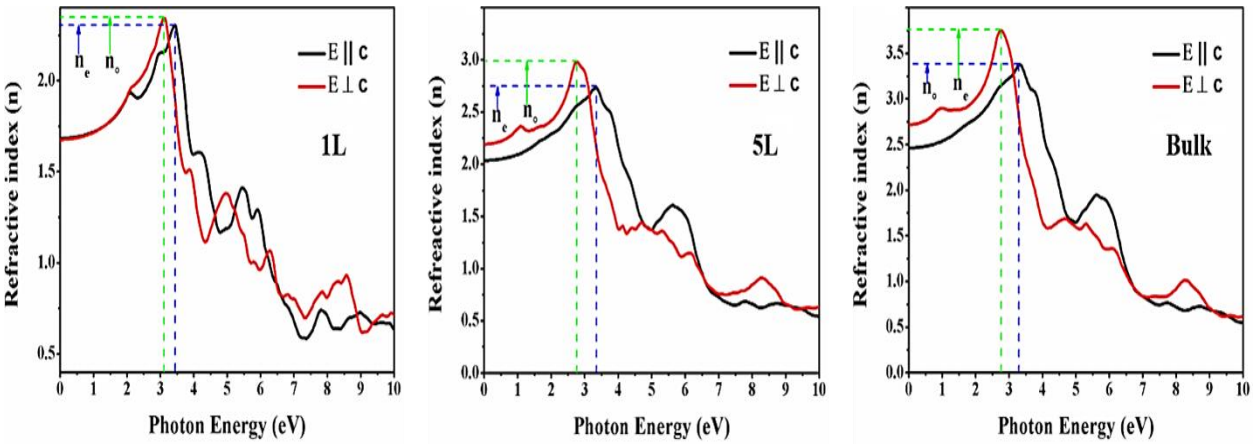

Figure S7: Calculated refractive index (n) along x and z directions for β-InSe monolayer (1L), few-layer (5L) and bulk β-InSe.