Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Insights into Electron Dynamics in Two-Dimensional Bismuth Oxyselenide: A Monolayer-Bilayer Perspective

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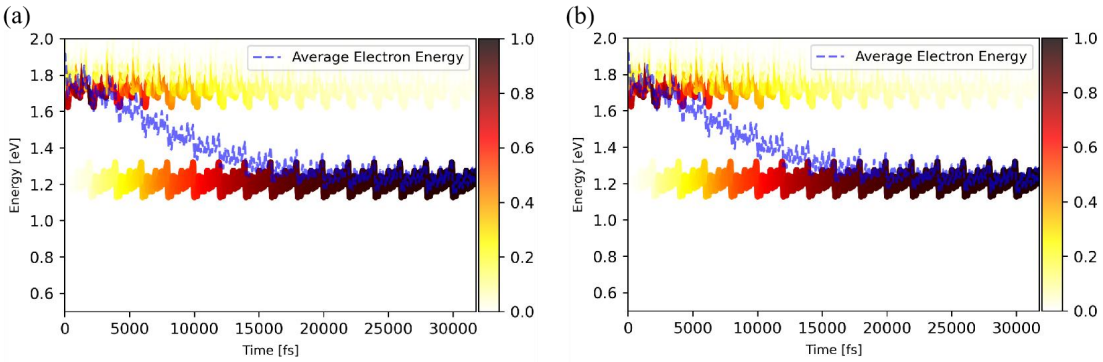

Figure S1. Time-dependent electron energy change of monolayer Bi_2O_2Se for (a) 100 samples and (b) 300 samples.

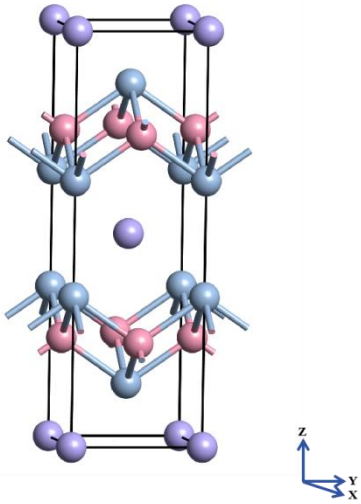

Figure S2. Schematic view of the structure of the bulk Bi_2O_2Se.

Table S1. Lattice parameters of monolayer and bilayer Bi_2O_2Se.

Lattice parameters	a	b	c	alpha	beta	gamma
Monolayer	3.92306	3.92306	20.00000	90.0000	90.0000	90.0000
Bilayer	3.92306	3.92306	40.00000	90.0000	90.0000	90.0000

Table S2. Electron effective masses for monolayer and bilayer Bi_2O_2Se.

Electron effective mass	m_e^{x*}	m_e^{y*}
Monolayer	0.17 m_0	0.17 m_0
Bilayer	0.12 m_0	0.12 m_0

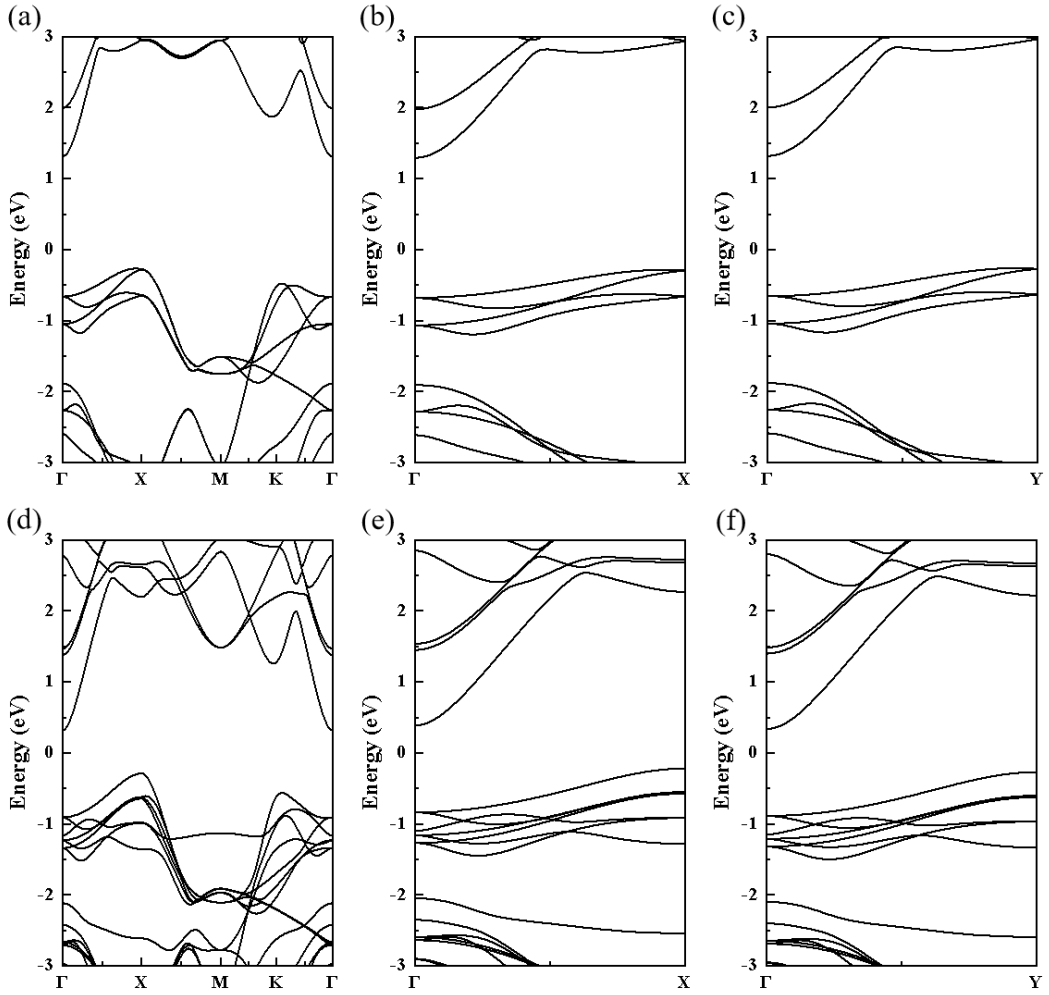

Figure S3. Band structures of (a-c) monolayer and (d-f) bilayer Bi_2O_2Se under different **k**-point paths.

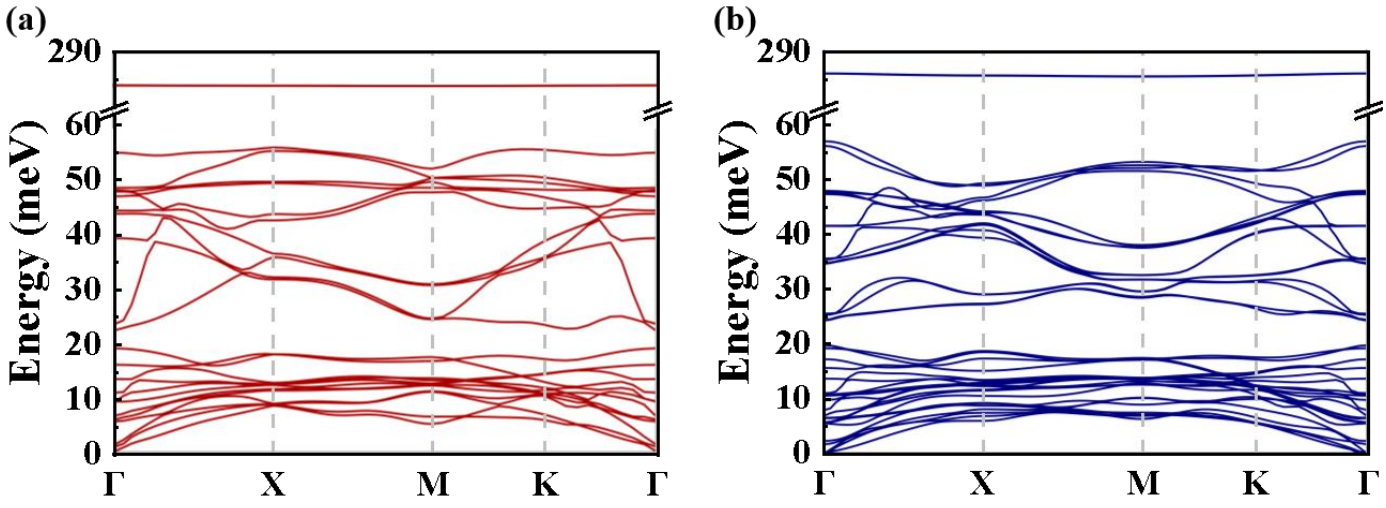

Figure S4. Phonon dispersions of (a) monolayer and (b) bilayer Bi_2O_2Se.

Table S3. Calculated bader charges for monolayer and bilayer Bi_2O_2Se.

Monolayer		charge/*e*	ZVAL	valence
	Bi	13.34	15.00	1.66
	O	7.17	6.00	-1.17
	Se	6.42	6.00	-0.42
	H	1.07	1.00	-0.07
Bilayer				
	outer Bi	13.35	15.00	1.65
	inner Bi	13.37	15.00	1.63
	O	7.16	6.00	-1.16
	outer Se	6.42	6.00	-0.42
	inner Se	6.95	6.00	-0.95
	H	1.07	1.00	-0.07

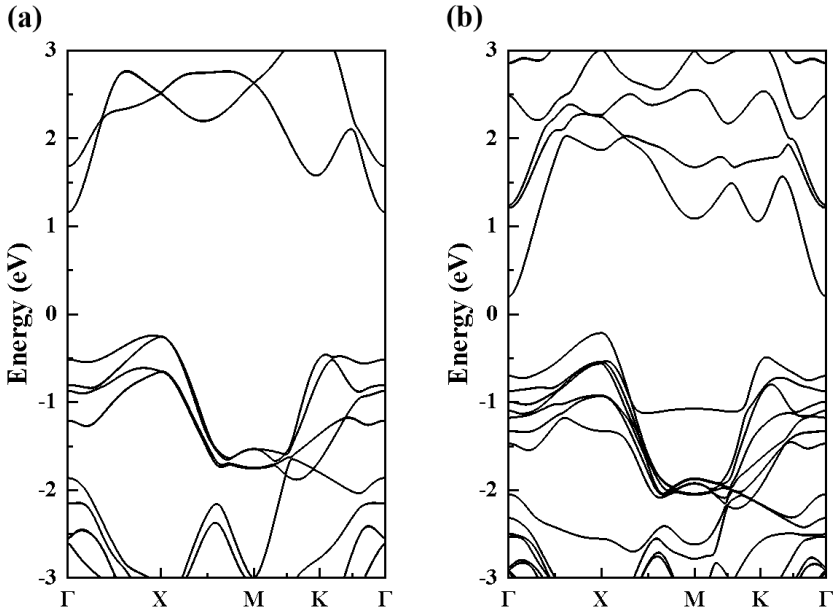

Figure S5. Band structures of (a) monolayer and (b) bilayer Bi_2O_2Se with SOC.

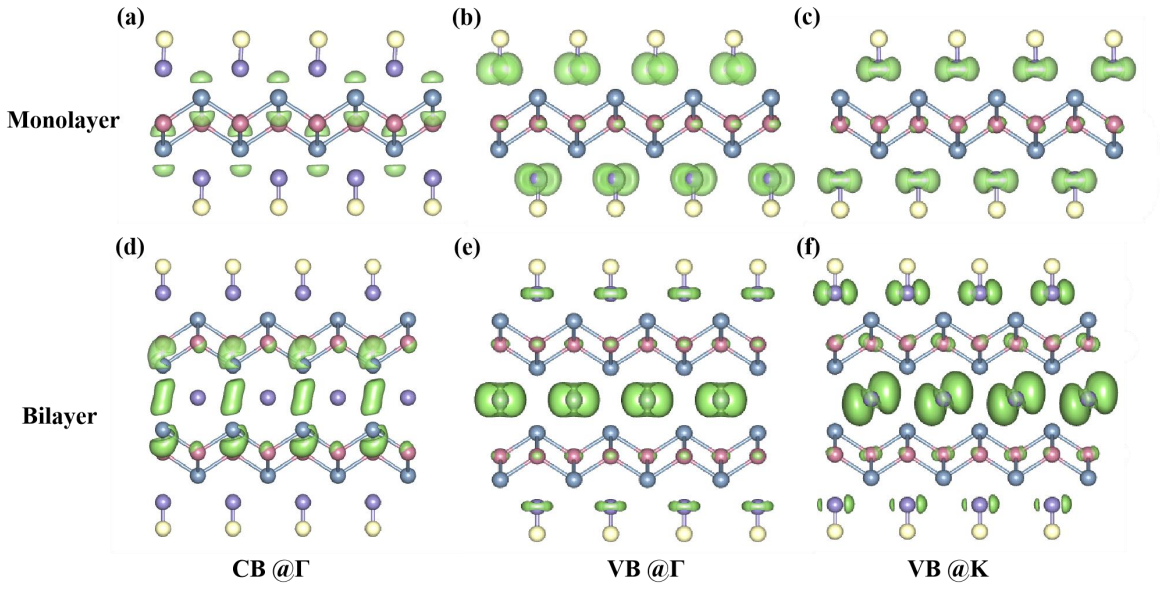

Figure S6. Partial charge density of monolayer and bilayer Bi_2O_2Se with SOC at the Γ point of the CBM, at the Γ point of the valence band and at the K point at the next highest position in the valence band.

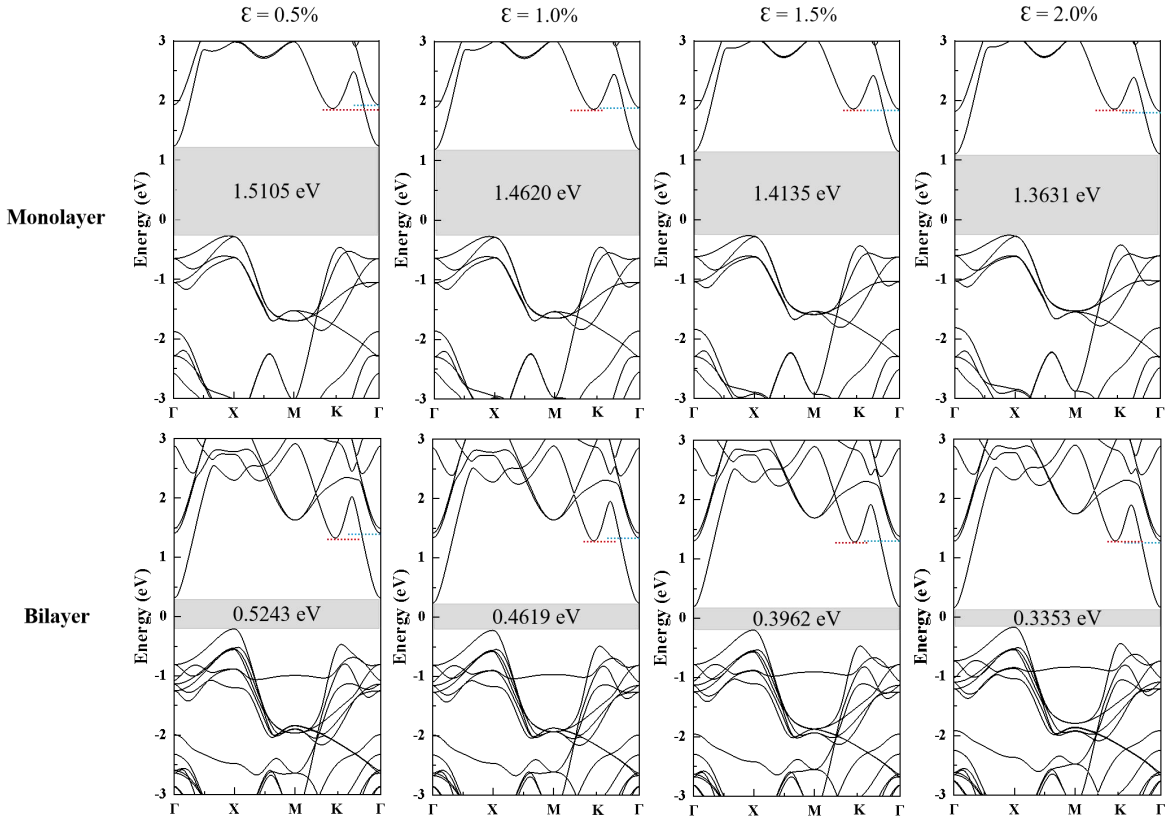

Figure S7. Band structures of monolayer and bilayer Bi_2O_2Se under 0.5, 1.0, 1.5, 2% strain calculated by DFT.