Supplementary Information

A DFT-NEGF study on the electronic and transport properties of 2D $SbSiTe_3$

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Table S1. The optimized lattice parameters, layered thickness (L), and interlayer distance (d_0) for few-layer $SbSiTe_3$.

Type	Lattice parameters (Å)	L (Å)	d_0 (Å)
Bulk	a=b=7.147	3.953	3.161
Five-layer	a=b=7.141	3.956	3.168
Four-layer	a=b=7.139	3.958	3.169
Trilayer	a=b=7.138	3.959	3.175
Bilayer	a=b=7.133	3.963	3.175
Monolayer	a=b=7.127	3.973	/

Table S2. The binding energy of few-layer and bulk $SbSiTe_3$.

Type	Binding Energy (eV/atom)
Bulk	4.210
Five-layer	4.191
Four-layer	4.186
Trilayer	4.178
Bilayer	4.162
Monolayer	4.118

Table S3. The off-current (I_{off}) and the on-current (I_{on}) of 2D $SbSiTe_3$ MOSFET with the channel length is 10 nm and 5nm.

Type	Channel length (nm)	V_{dd}	I_{off} (μA/μm)	I_{on} (μA/μm)
	10	0.72	0.1	210
		0.72	2×10^{-5}	30

n-type	5	0.64	0.1	51
		0.64	5×10^{-5}	\
p-type	10	0.72	0.1	350
		0.72	2×10^{-5}	32
	5	0.64	0.1	223
		0.64	5×10^{-5}	\

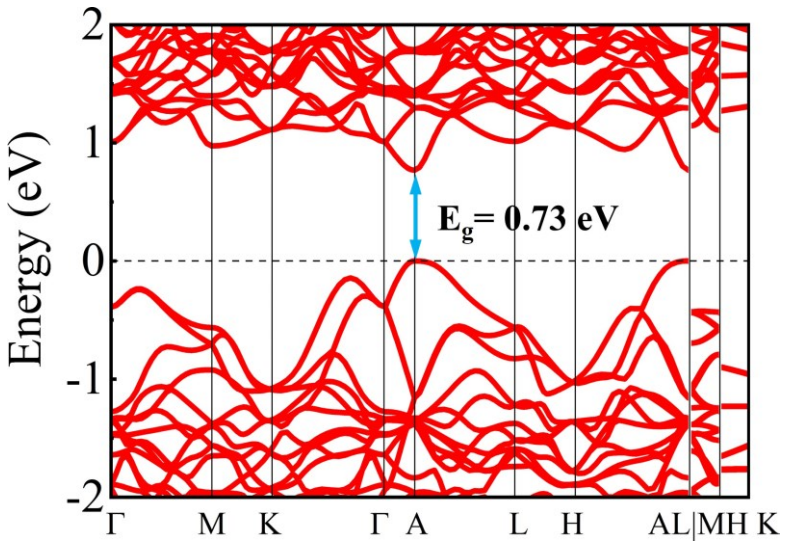

Fig. S1. The band structure of bulk $SbSiTe_3$ at HSE06 level.

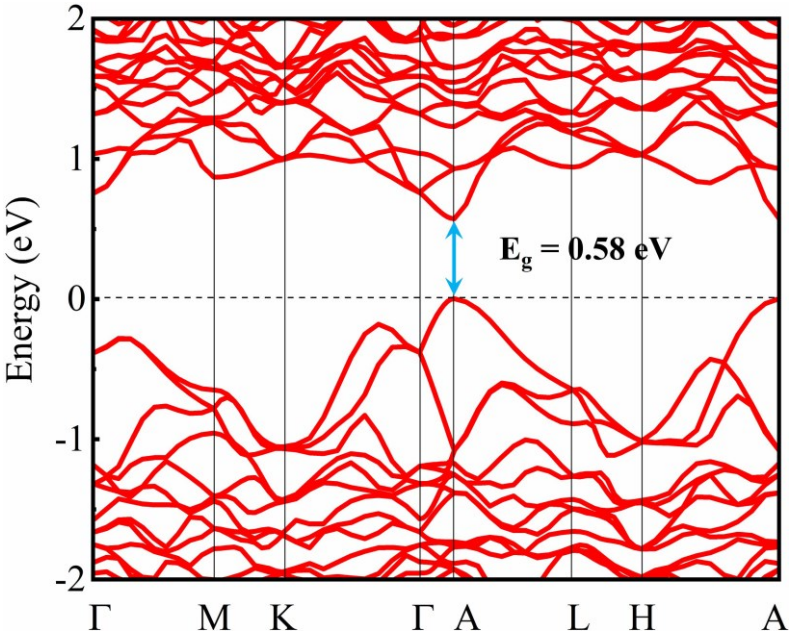

Fig. S2. The band structure of bulk $SbSiTe_3$ at HSE06+soc level.

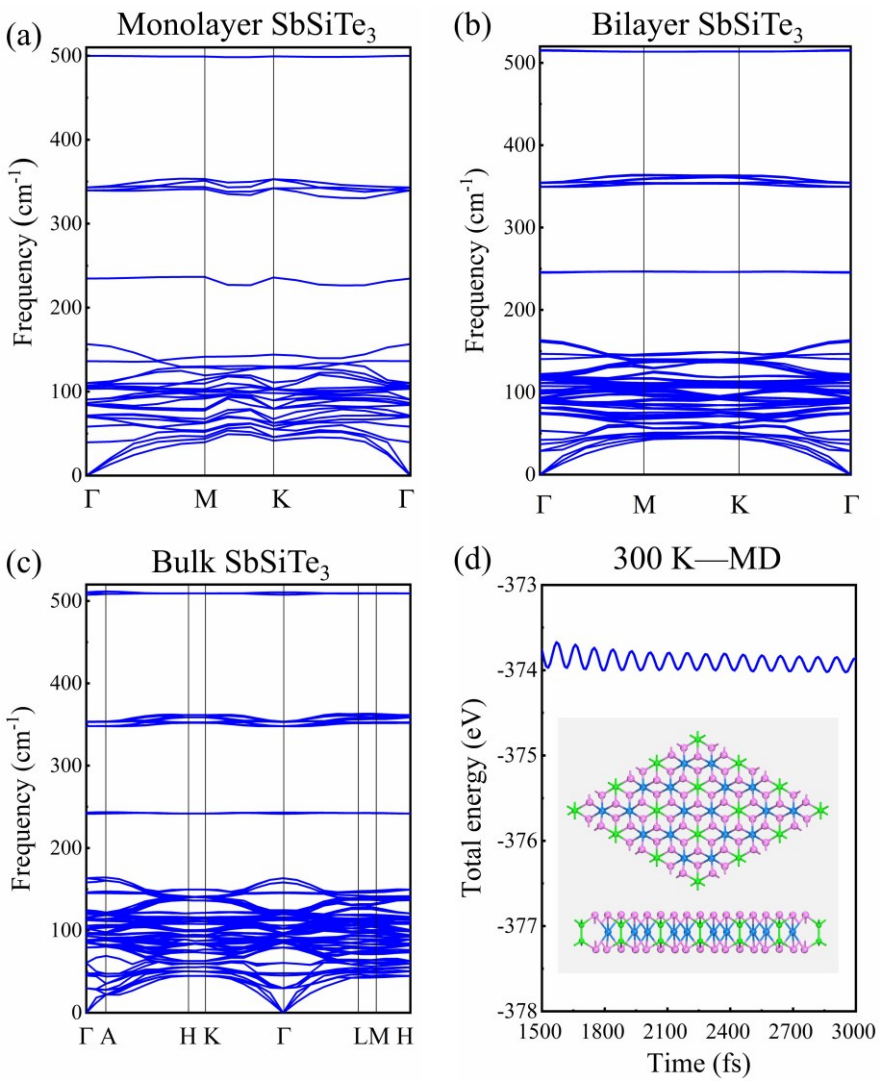

Fig. S3. The phonon spectrums of (a) monolayer, (b) bilayer and (c) bulk $SbSiTe_3$. (d) The total energy variation versus time at T = 300 K, and insert is the top and side views of a snapshot of monolayer $SbSiTe_3$ after 3 ps in the MD simulation.

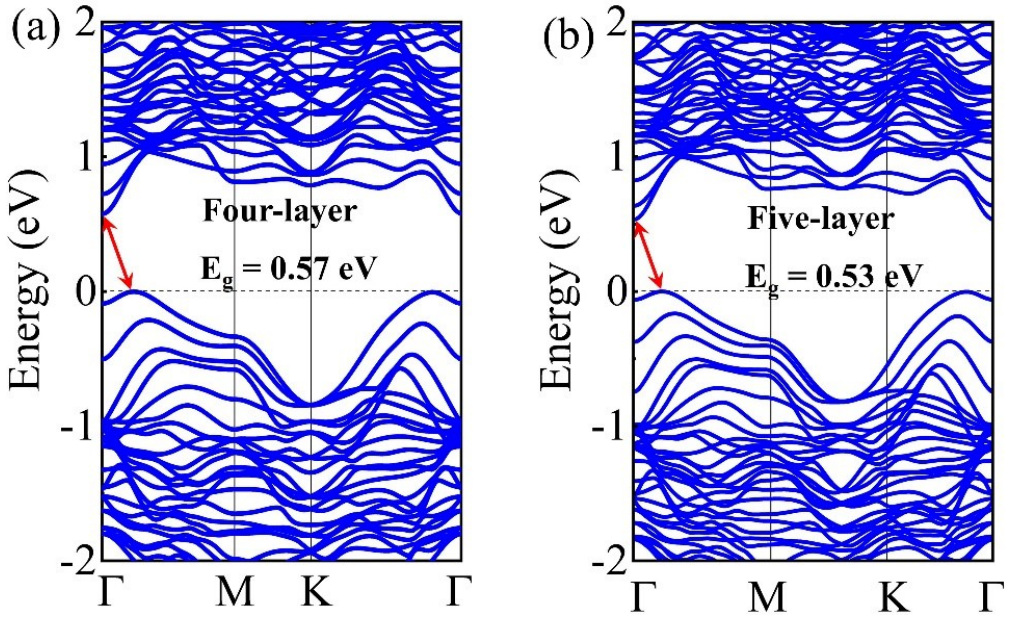

Fig. S4. The band structures of (a) four-layer and (b) five-layer $SbSiTe_3$ at PBE level.

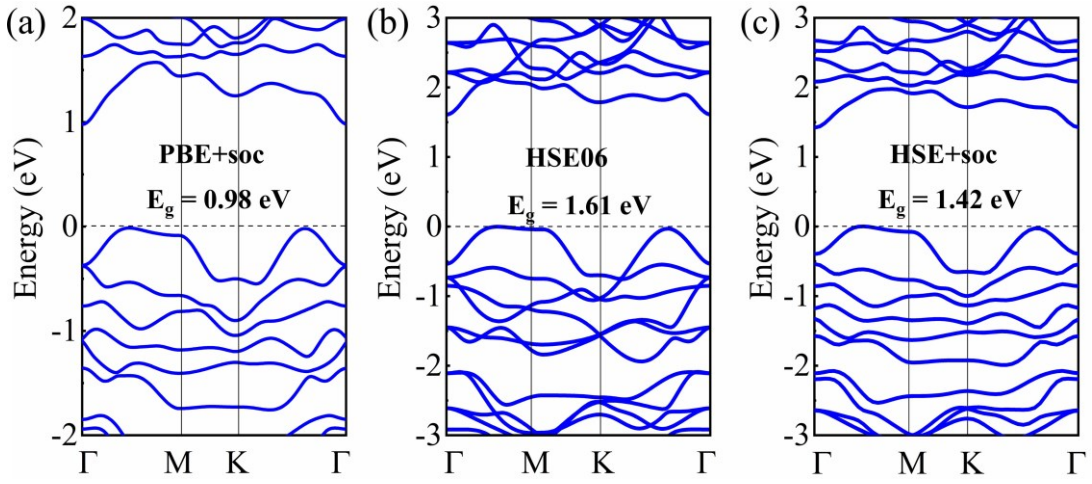

Fig. S5. The band structure of monolayer $SbSiTe_3$ at (a) PBE + soc, (b) HSE06 and (c) HSE + soc level.

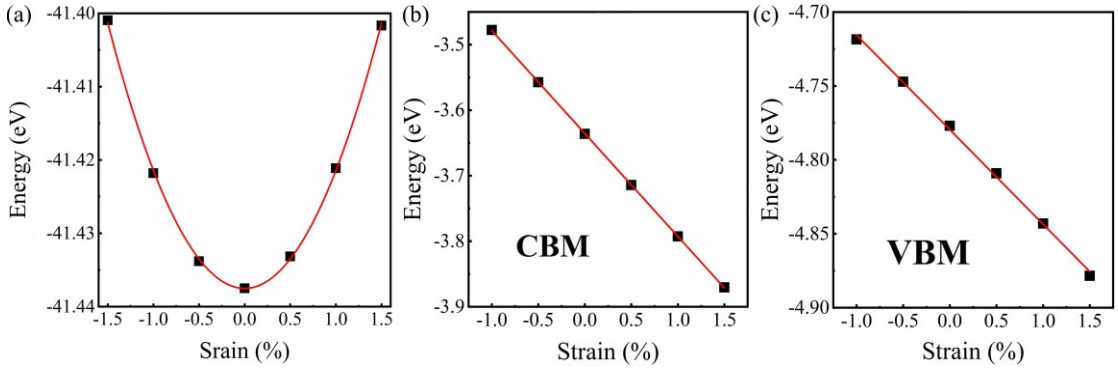

Fig. S6. (a) The energy-strain relation and the energy shifts versus strain with respect to the vacuum energy of (b) CBM and (c) CBM for monolayer $SbSiTe_3$.