Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Material for

Two-dimensional GeAsSe with High and Unidirectional Conductivity

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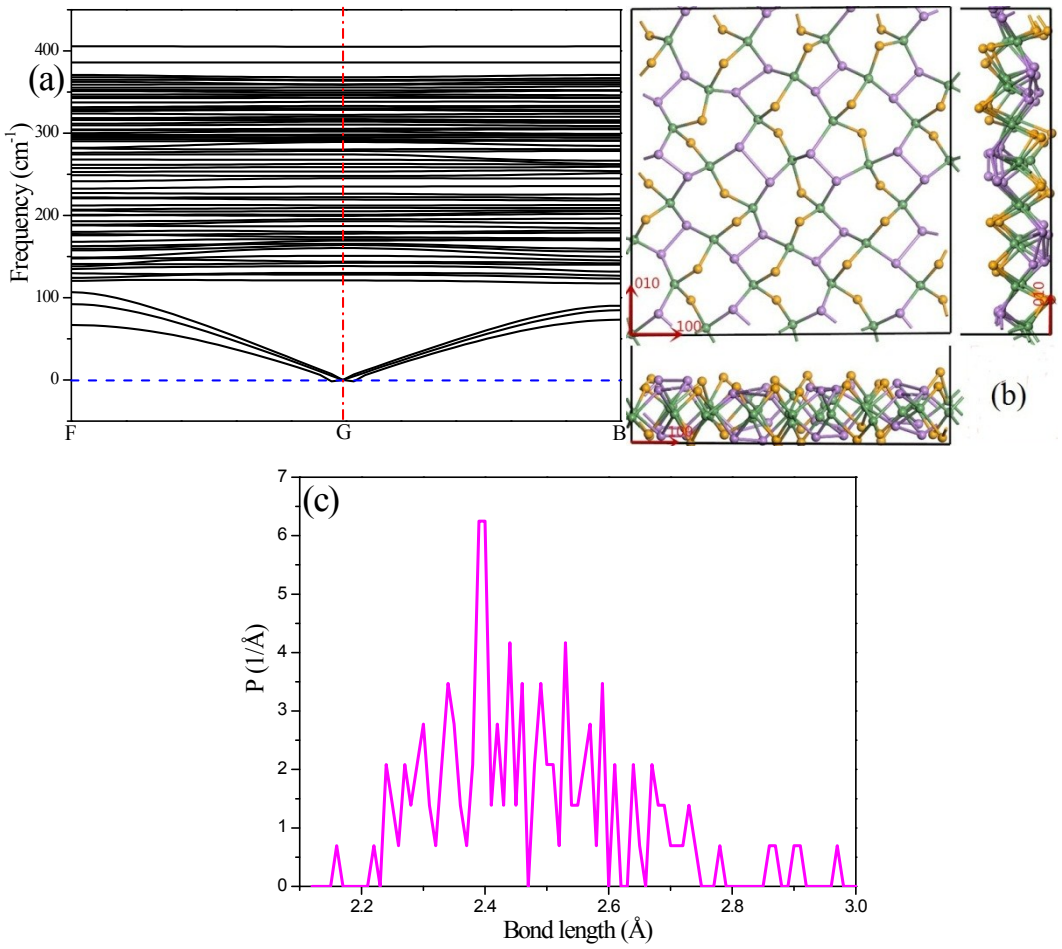

Figure s1. (a) The phonon dispersion curves of monolayer GeAsSe. **(b)** Top and side views of an

AIMD snapshot of monolayer GeAsSe at 1300 K. **(c)** The distribution of the bond length after AIMD simulation. The phonon dispersions of monolayer GeAsSe are calculated to test the kinetic stability. The thermal stability of GeAsSe is further investigated by ab initio molecular dynamics (AIMD) simulation. A 4×2×1 GeAsSe supercell (contains 96 atoms) remains intact at 1300 K lasts for 3 ps with a time step of 1.0 fs, which is controlled by using the Nosé-Hoover thermostat.

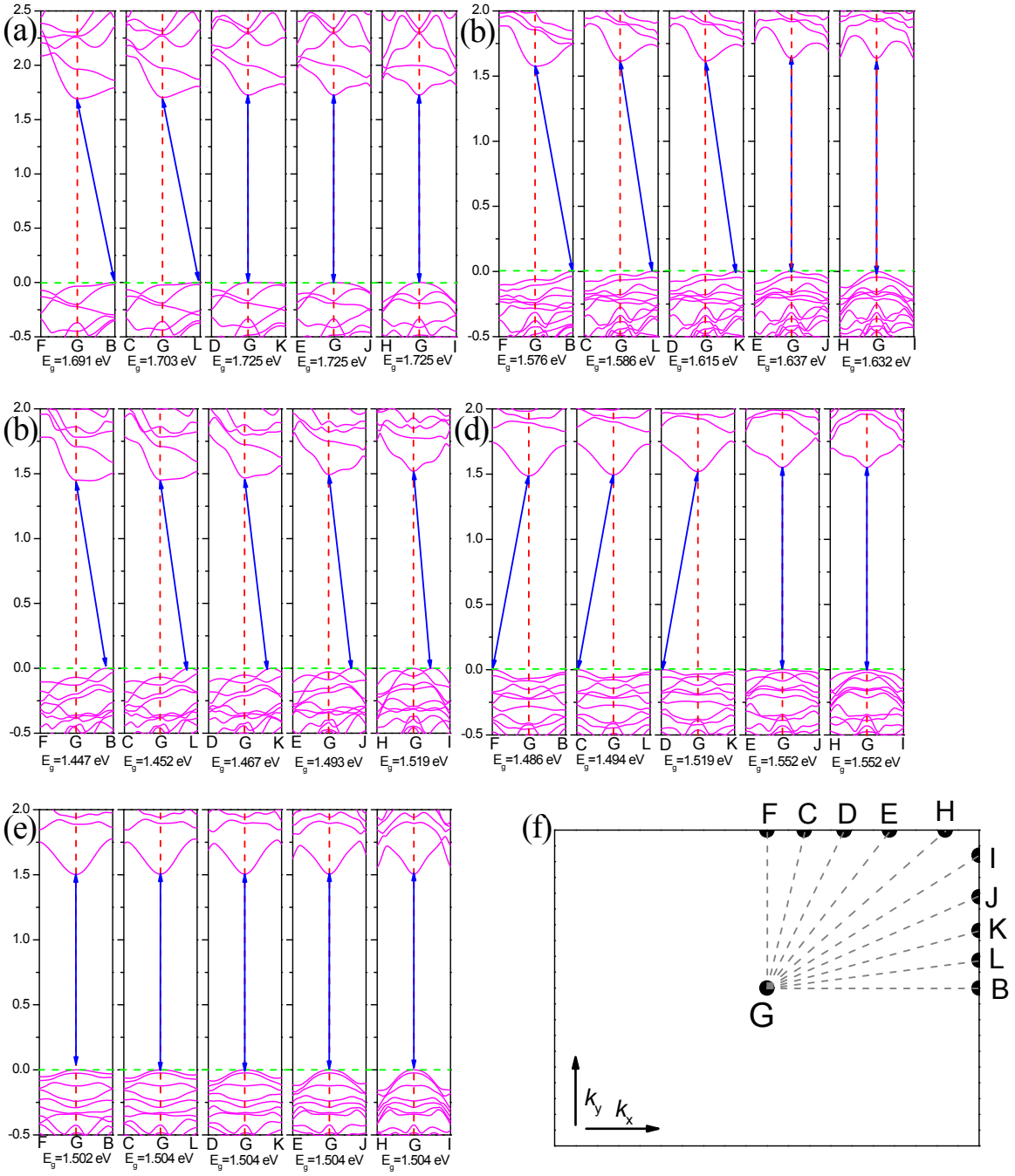

Figure s2. details of band structures in (a) monolayer and bilayer GeAsSe with stacking modes of

(b) type I, (c) type II, (d) type III and (e) type IV. (f) The first Brillouin zone. “G”, “F”, “C”, “D”, “E”, “H”, “I”, “J”, “K”, “L”, “B” represent the Brillouin zone points.

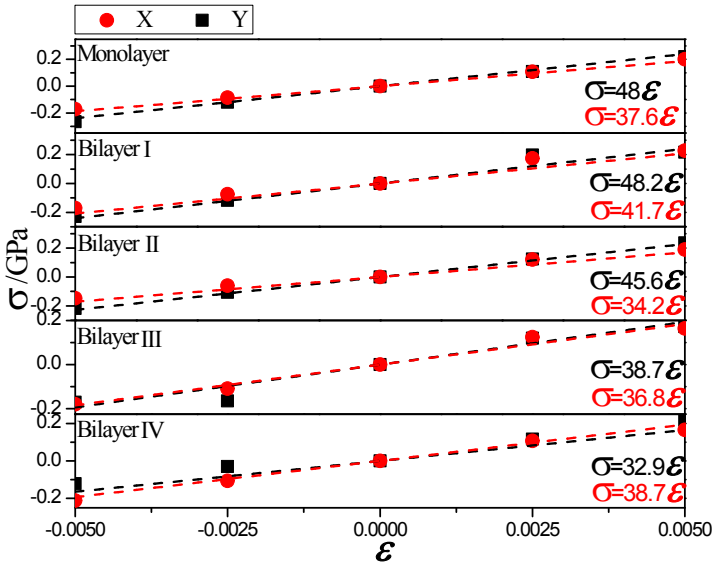

Figure s3. Axial stresses of monolayer or bilayer GeAsSe with respect to the uniaxial stretching and compression along the x (100) or y (010) directions. Dash lines represent the linear fitted results.

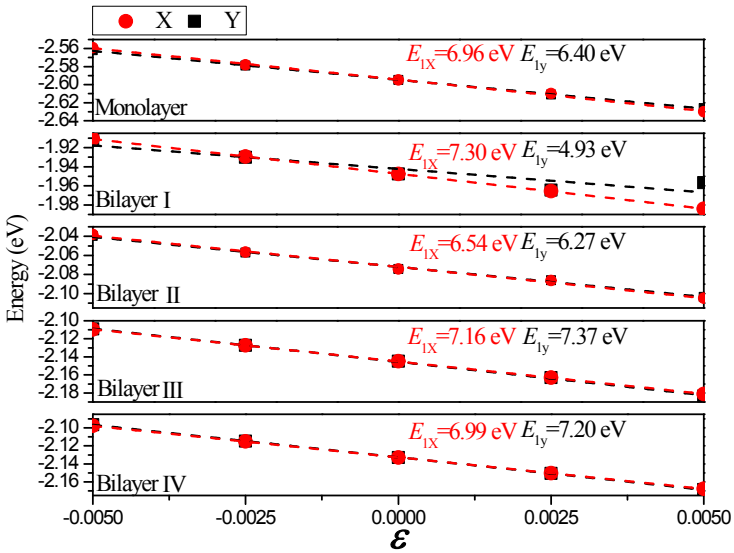

Figure s4. Energy shift of CBM for monolayer or bilayer GeAsSe with respect to the lattice dilation and compression along the X and Y directions, respectively.

Table s1. Lattice parameters, Van der Waals (vdW) gap, binding energy and band gap of single or

double layered GeAsSe calculated by PBE+D.

	Single layer	Double layers			
		type I	type II	type III	type IV
Lattice a/b (Å)	10.19/10.44	10.06/10.39	10.09/10.46	10.27/10.29	10.29/10.28
vdW gap (Å)	–	2.84	2.62	3.12	3.10
Binding energy (meV/Å^2)	–	-0.62	0.97	11.50	8.64
Band gap (PBE+D, eV)	1.69	1.58	1.45	1.49	1.50

Table s2. The in-plane stiffness C_{2D}, DP constant E_1, effective mass m_e and carrier mobility $\boldsymbol{\mu}$ at 300K for monolayer and bilayer GeAsSe along X (100) direction and Y (010) directions.

	Monolayer		Bilayer							
			I		II		III		IV	
	X	Y	X	Y	X	Y	X	Y	X	Y
C_{2D} (N/m)	23.30	28.30	51.58	56.87	42.83	53.14	44.54	46.66	46.7	39.78
E_1 (eV)	6.96	6.40	7.30	4.93	6.54	6.27	7.16	7.37	6.99	7.20
m_e (m_0)	2.04	0.38	2.3	0.42	3.85	0.32	0.55	0.57	0.52	0.62
$\boldsymbol{\mu}$ (cm^{2}v^{-1}s^{-1})	1.60	70.0	2.60	188.15	0.96	192.02	41.04	36.89	49.76	28.70

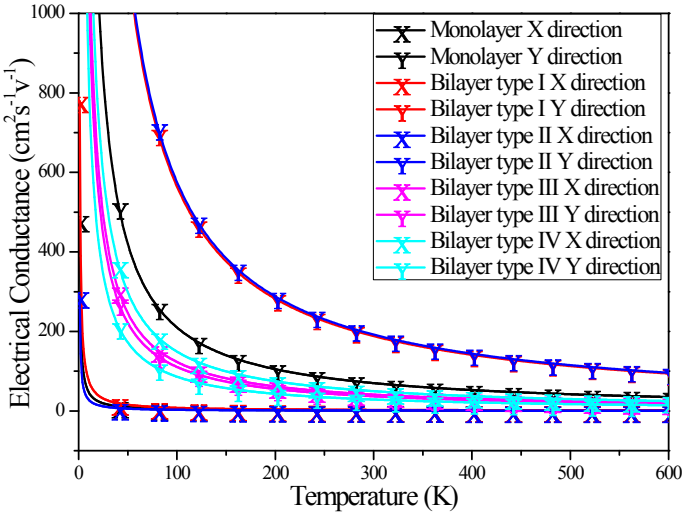

Figure s5. The electrical mobility of monolayer and bilayer GeAsSe considering temperature effects.

Table s3. The lattice parameters, vdW gap, binding energy and band gap of single and double layers calculated with PBE method.

	Single layer	Double layers

		type I	type II	type III	type IV
Lattice *a*/*b* (Å)	10.19/10.44	10.13/10.42	10.15/10.49	10.33/10.33	10.34/10.33
vdW gap (Å)	–	2.86	2.64	3.12	3.09
Binding energy (meV/ Å^2)	–	-0.89	0.73	11.20	8.35
Band gap (PBE, eV)	1.69	1.52	1.41	1.44	1.46

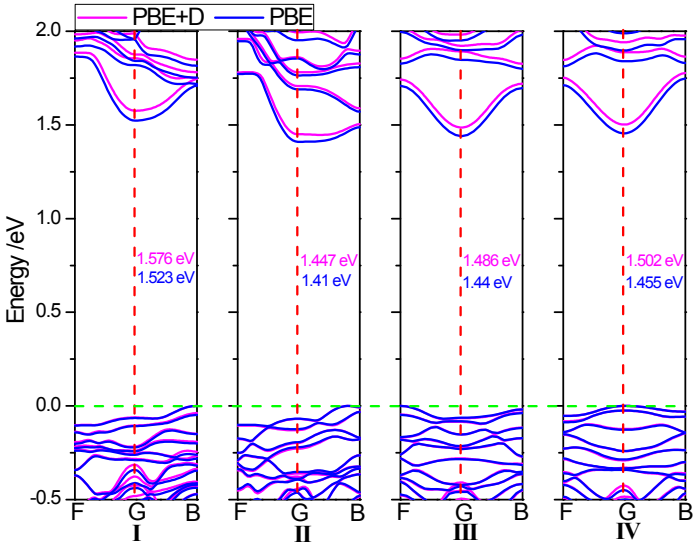

Figure s6. The band structure of bilayer GeAsSe calculated with PBE (blue lines) and PBE+D (magenta lines) method.