Supplementary information

for

Strain-engineering the electrical anisotropy of GeSe monolayer

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Fig. S1.

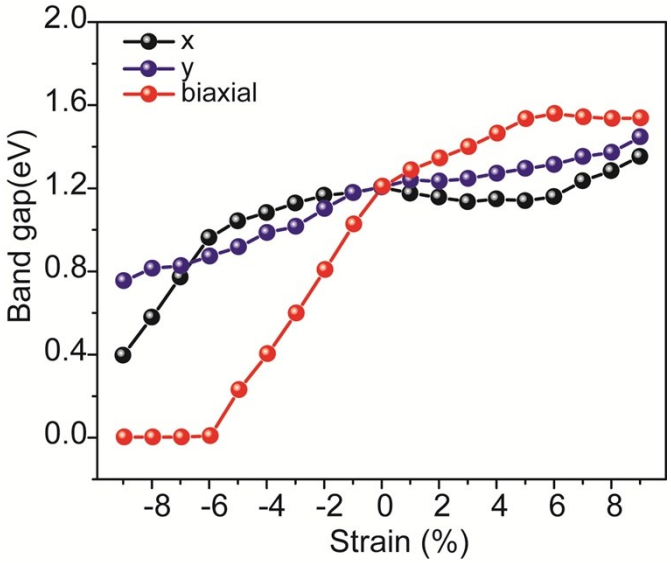

Fig. S1 Calculated band gap of GeSe monolayer under different strains.

Fig. S2

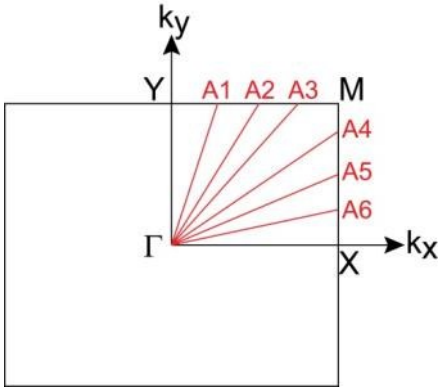

Fig. S2 Brillouin zone path adopted for the polar plots of the anisotropic effective mass.

Fig. S3

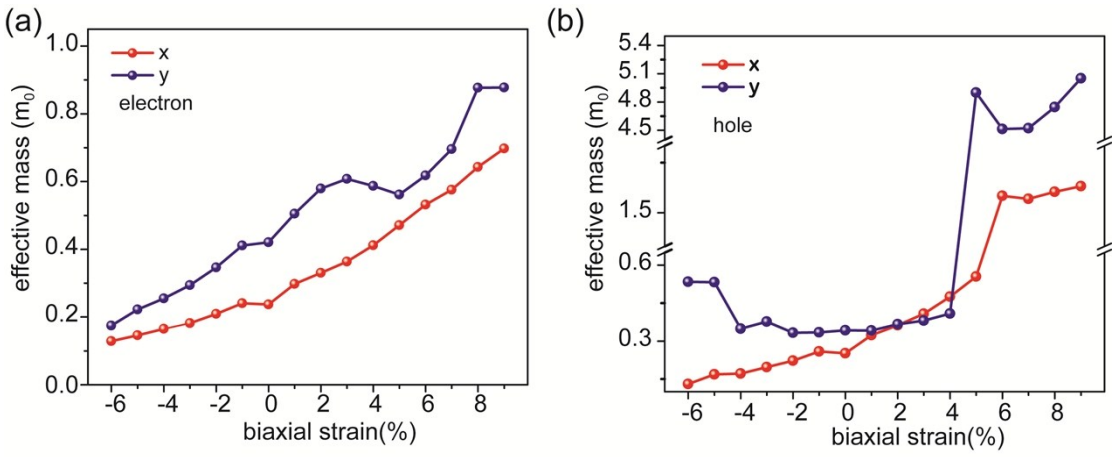

Fig. S3 Effective masses of electron and hole under different biaxial strain.

Fig. S4

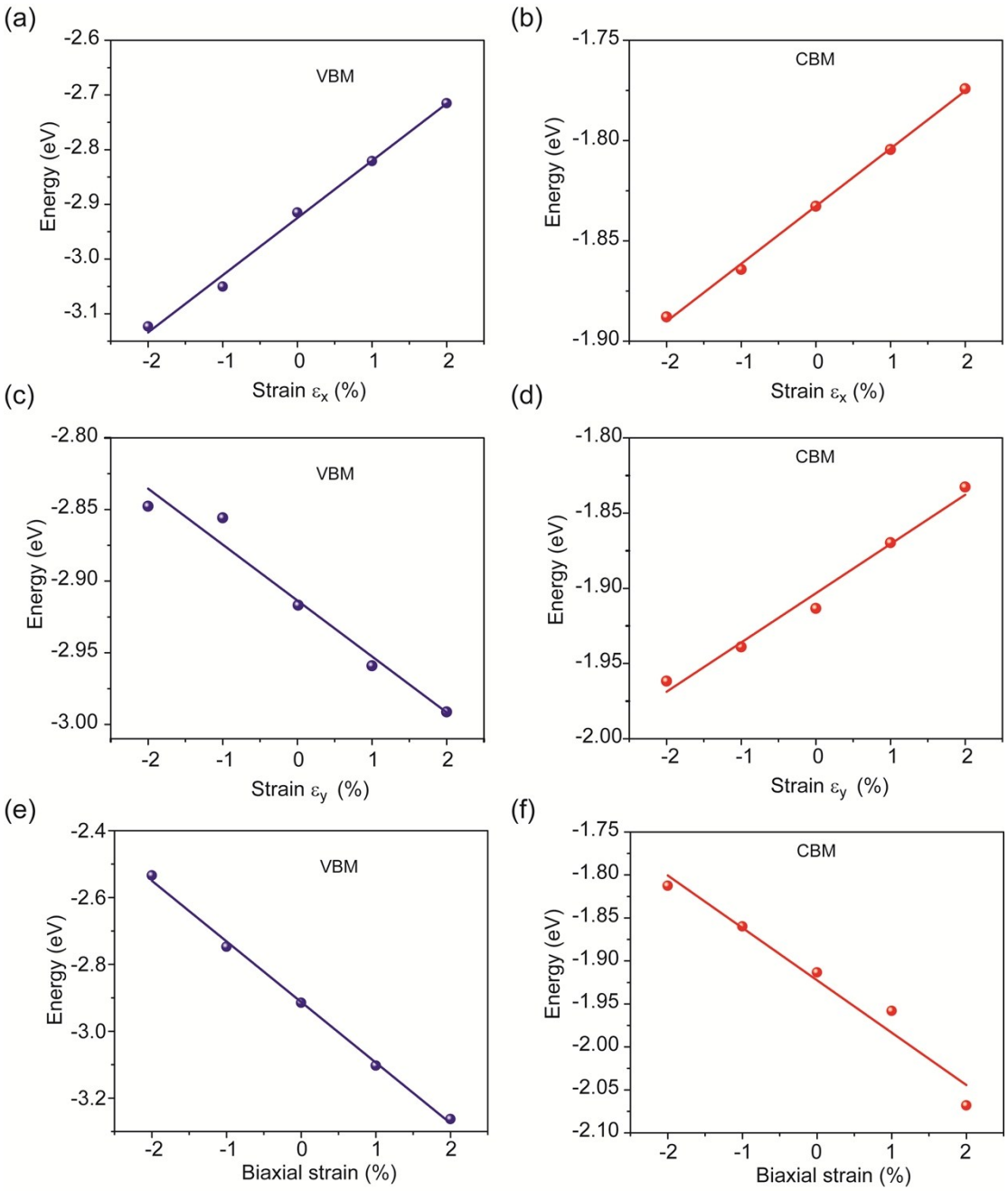

Fig. S4 Fermi level shift with respect to the lattice dilation $\Delta l/l_0$ along different directions. Linear fit of the data gives the DP constant.

Fig. S5

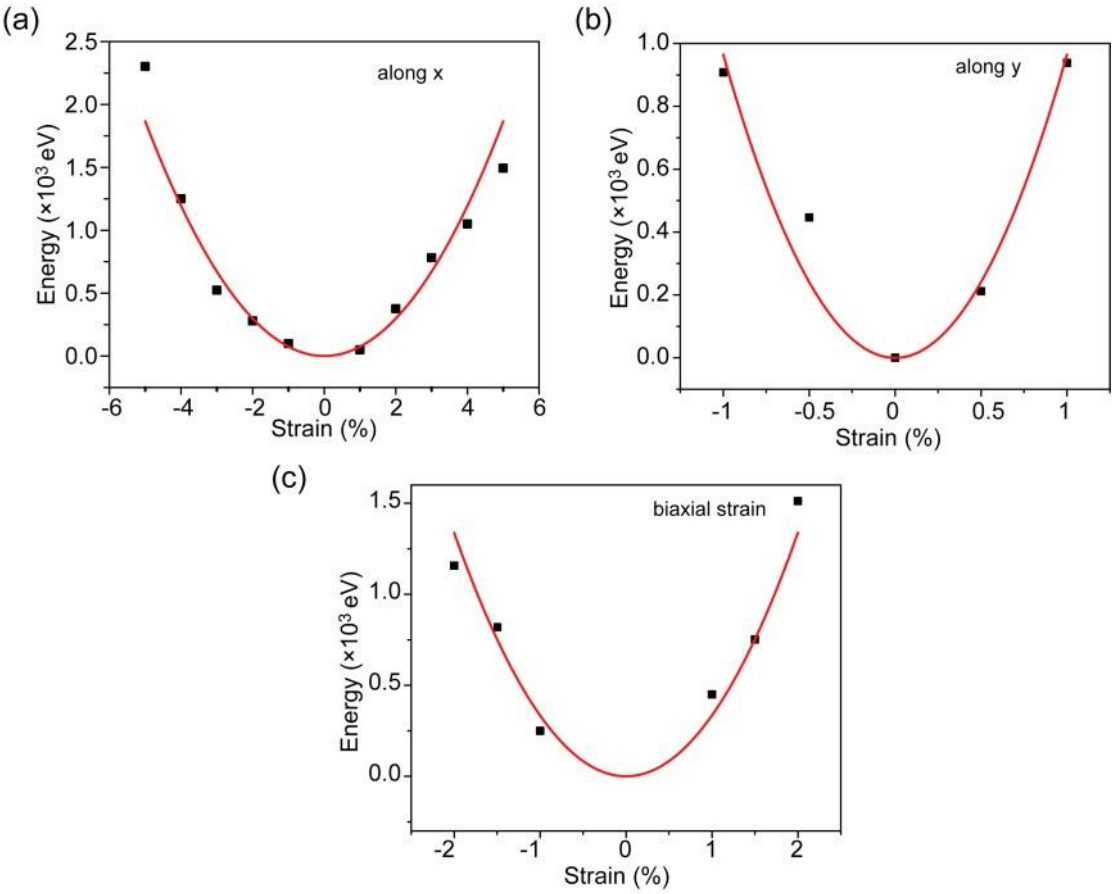

Fig. S5 Evolution of total energy with respect to the lattice dilation $\Delta l/l_0$ along different directions. Quadratic fit of the data gives the 2D elastic constant.

Fig. S6

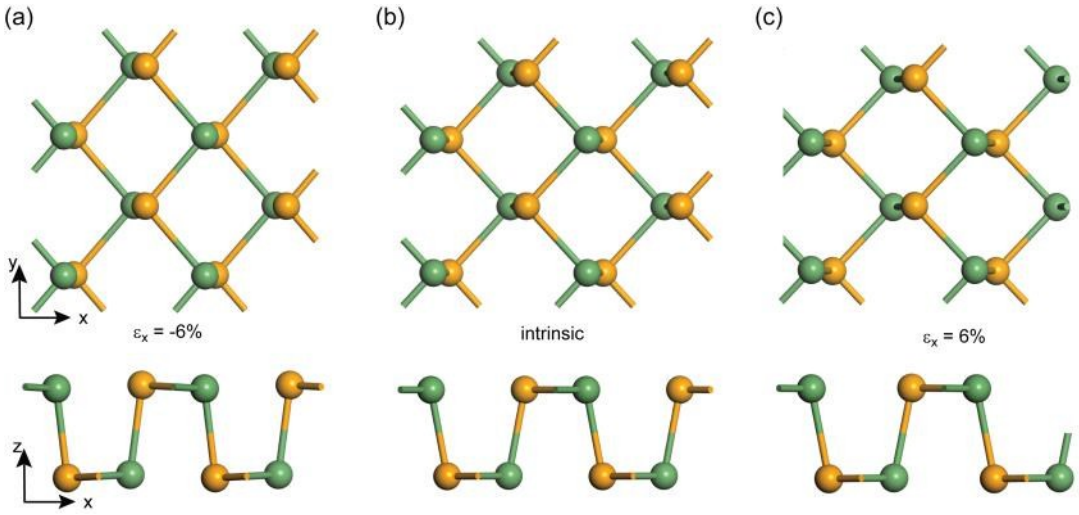

Fig. S6 Configuration of GeSe monolayer under strains along armchair. (a) Compression with ε_x = -6%. (b) Optimized structure without strain. (c) Tension with ε_x = 6%. Top and side views are displayed in all panels.

Fig. S7

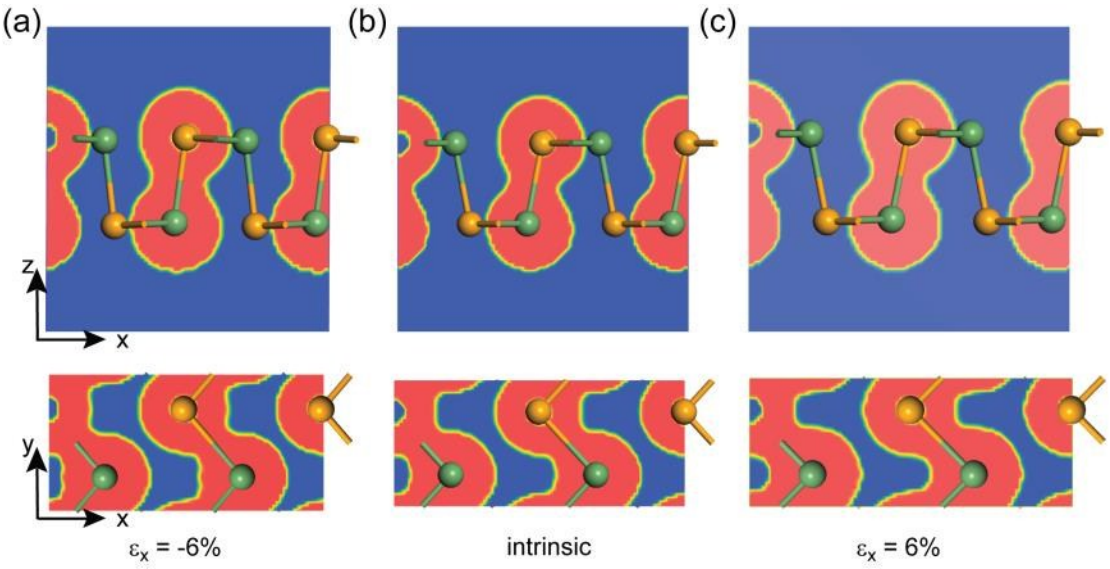

Fig. S7 Charge density of Ge-Se bond b_{13} (top) and b_{34} (down) under strains along armchair. (a) Compression with $\varepsilon_x = -6\%$. (b) Optimized structure without strain. (c) Tension with $\varepsilon_x = 6\%$. The iso-value of the charge density is 0.005 e Å^{-3}.

Table S1

Table S1 Lattice constants of intrinsic bulk GeSe

lattice constants			band gap	
a (Å)	b (Å)	c (Å)	(eV)	
4.41	3.84		1.16	Ref. R1
4.39	3.90	10.93		Ref. R2
4.378	3.839	10.84	1.14, 1.20	Ref. R3, R4 (Exp.)
4.46	3.848	10.96	0.907/1.252	Our results(PBE/HSE06)

R1 Y. H. Hu, S. L. Zhang, S. F. Sun, M. Q. Xie, B. Cai and H. H. Zeng, *Appl. Phys. Lett.* 2015, **107**, 122107.

R2 L. C. Gomes, A. Carvalho and A. H. Castro Neto, *Phys. Rev. B*, 2016, 94, 054103.

R3 D.-J. Xue, S.-C. Liu, C. M. Dai, S. Chen, C. He, L. Zhao, J.-S. Hu and L. J. Wan, *J. Am. Chem. Soc.*, 2017, **139**, 958-965.

R4 P. D. Antunez, J. J. Buckley and R. L. Brutchey, *Nanoscale*, 2011, **3**, 2399.

Table S2

Table S2 Selected bonds and angles of GeSe monolayer under different strains along armchair

	bond 1-3 (Å)	bond 3-4 (Å)	θ_{132} (°)	θ_{234} (°)
ε_x = -6%	2.6741	2.4909	98.661	96.198
intrinsic	2.6086	2.5117	94.968	96.932
ε_x = -6%	2.5587	2.5308	90.183	98.734