Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information

Germanium Monosulfide Monolayer: A Novel Two-Dimensional Semiconductor with High Carrier Mobility

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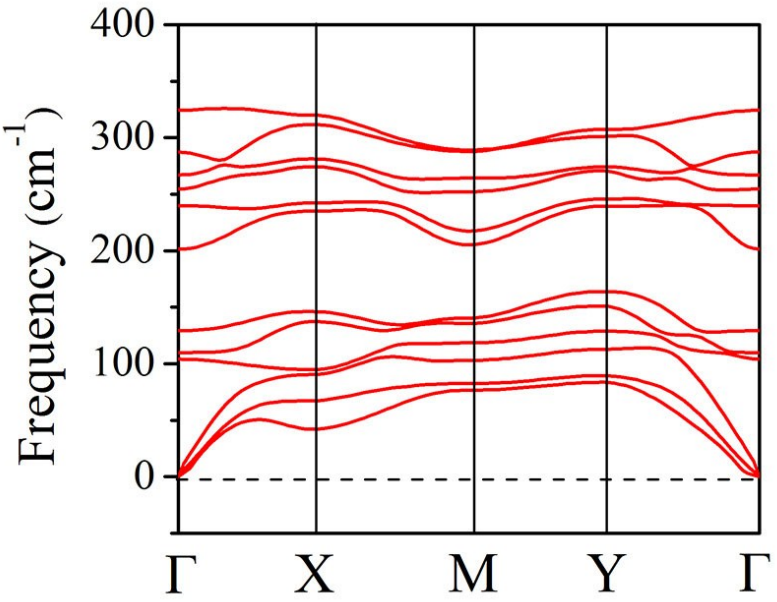

Fig. S1 Phonon spectrum of GeS monolayer.

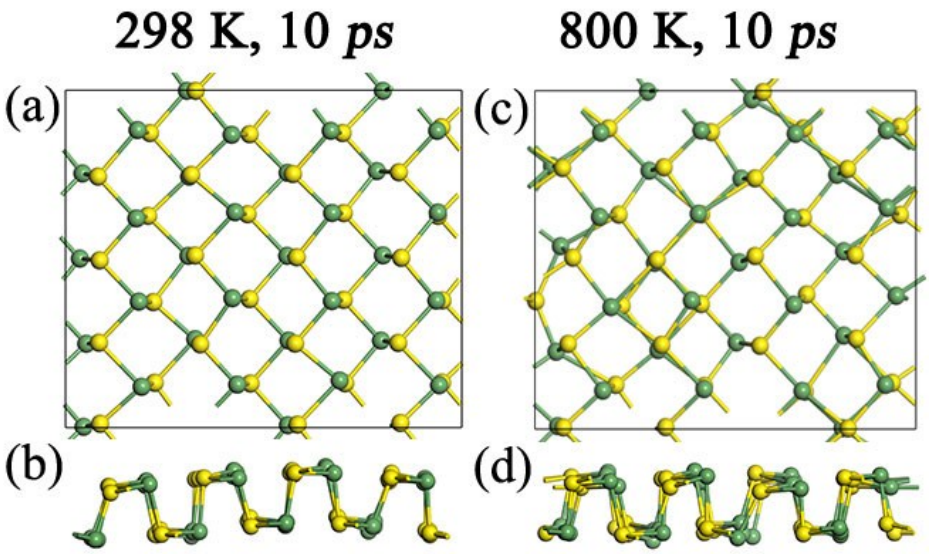

Fig. S2 Snapshots of the equilibrium structures of GeS monolayer at (a) 298 K, and (b) 800 K, respectively, at the end of 10 ps first-principles molecular dynamic (MD) simulation.

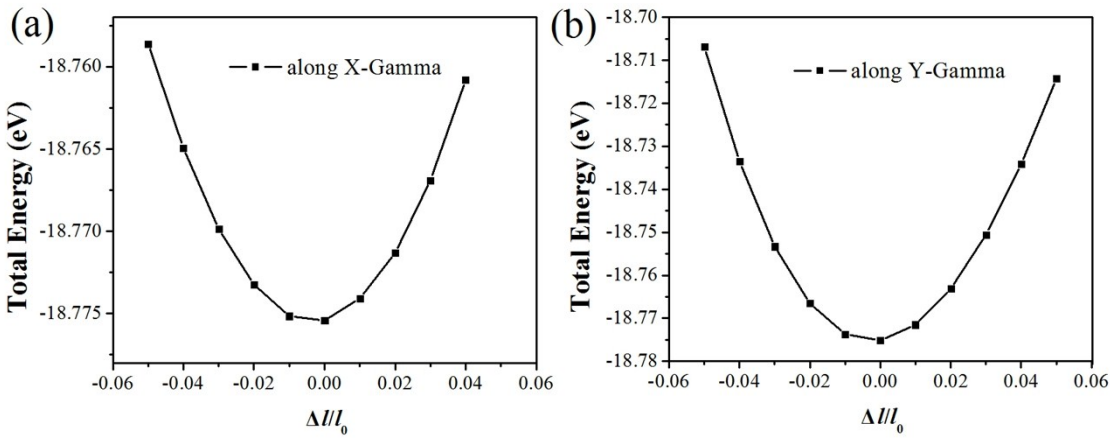

Fig. S3 Total energy-strain relationship of GeS monolayer along *x* (a) and *y* (b) directions. Δl refers to the dilation along *x* or *y*, while l_0 refers to the lattice constant of *a* or *b* at equilibrium geometry.

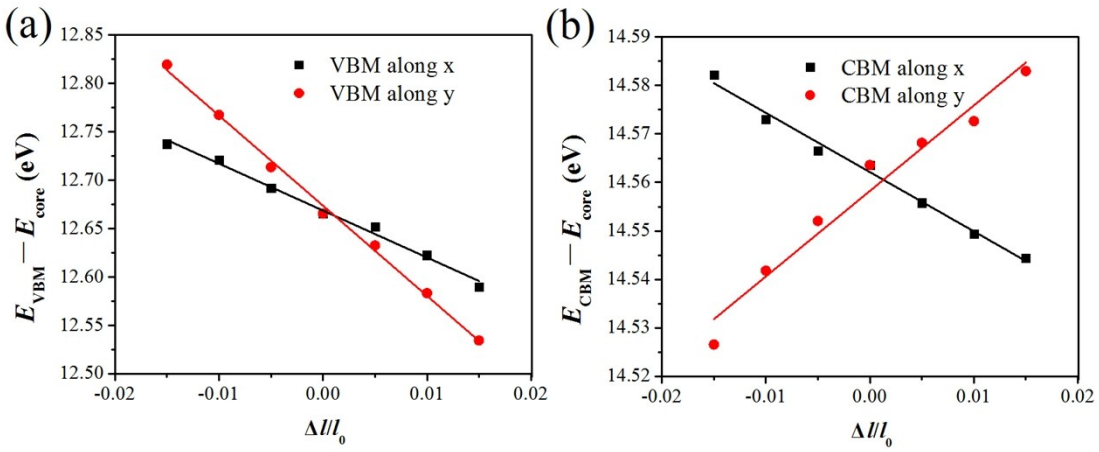

Fig. S4. Shifts of VBM and CBM under uniaxial strain along *x* and *y* directions for GeS monolayer.

TABLE. S1. At the PBE level, the carrier effective masses (m*), stretching modules (C), deformation potential constant (E_1), and carrier mobility (μ) of the investigated GeS monolayer.

Carrier Type	m^*/m_0	C (J m^{-2})	E_1 (eV)	μ (cm^2 v^{-1} s^{-1})
electron (x)	0.26	15.48	1.22	2.64×10^3
electron (y)	0.40	51.59	1.76	2.75×10^3
hole (x)	0.19	15.48	4.85	0.22×10^3
hole (y)	0.62	51.59	9.31	0.06×10^3