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

Supplementary Information

Structural stabilities, electronic structures, and superconductivity properties of Ge_xS_{1-x} compounds under high pressure

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Supporting Figures

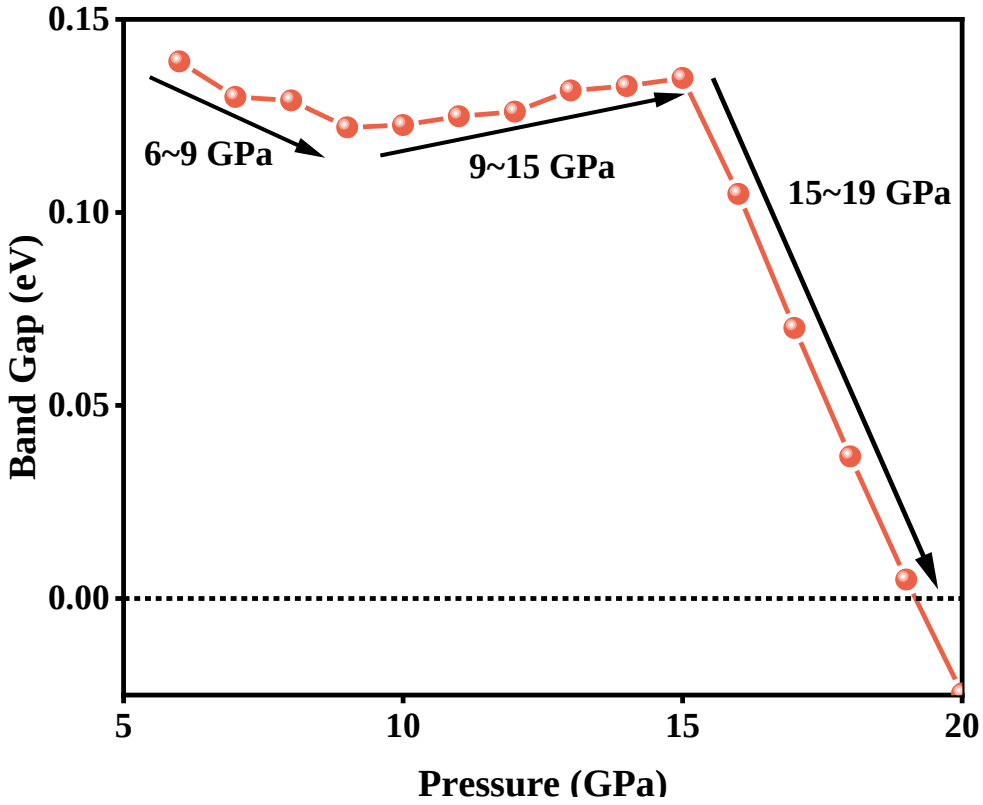

Fig. S1 Band gap changes of *Pnma*-2 GeS within 6~19 GPa.

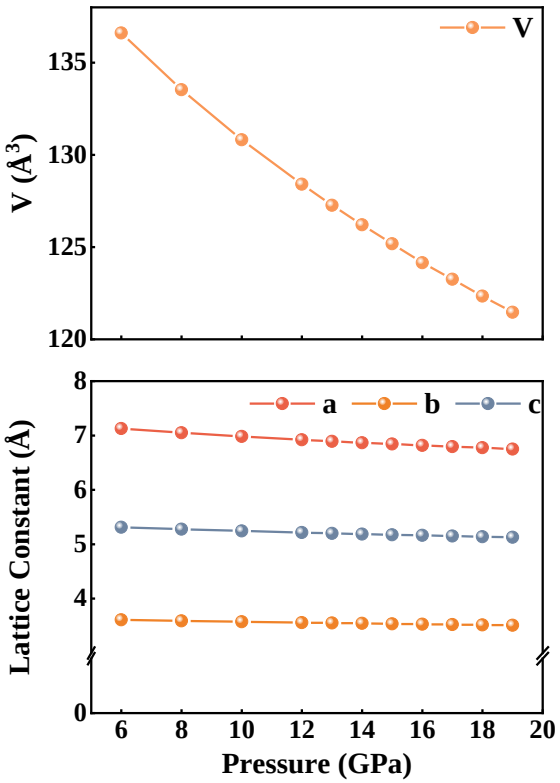

Fig. S2 Parameters of *Pnma*-2 within 6~19 GPa.

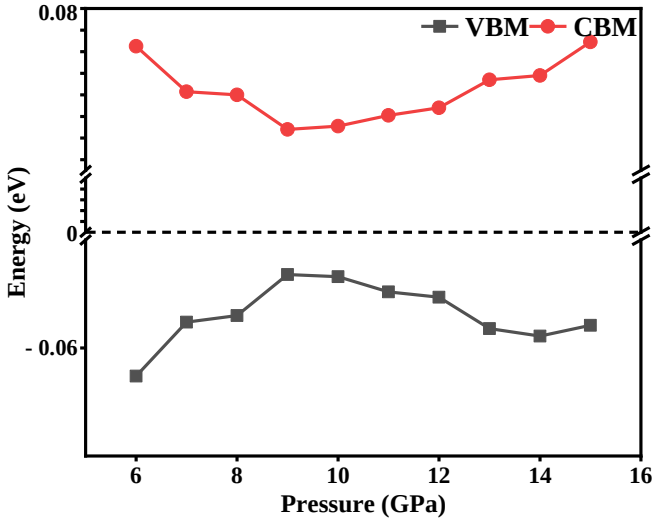

Fig. S3 VBM and CBM shifting within 6~15 GPa.

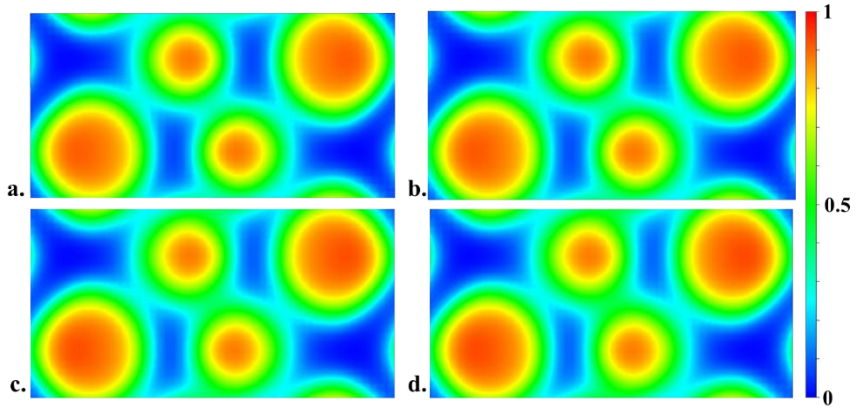

Fig. S4-A ELF of (0 0 1) plane of *Pnma*-2 at (a) 6 GPa, (b) 9 GPa, (c) 15GPa and (d) 19 GPa.

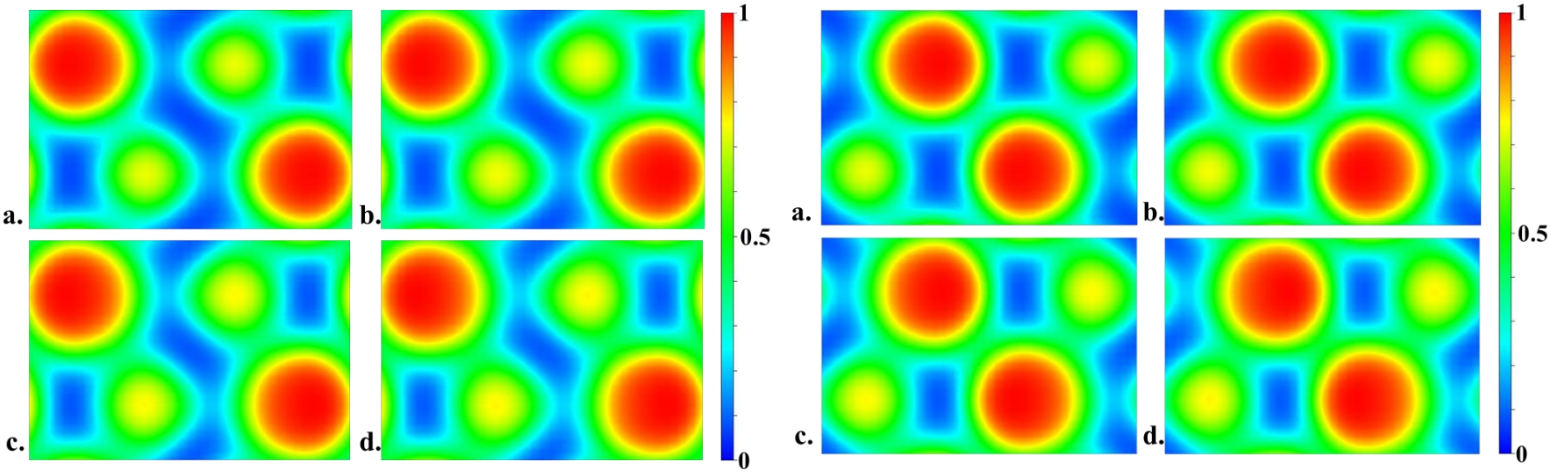

Fig. S4-B ELF of (1 0 0) plane of *Pnma*-2 at origin surface and middle sliced space under (a) 6 GPa, (b) 9 GPa, (c) 15GPa and (d) 19 GPa.

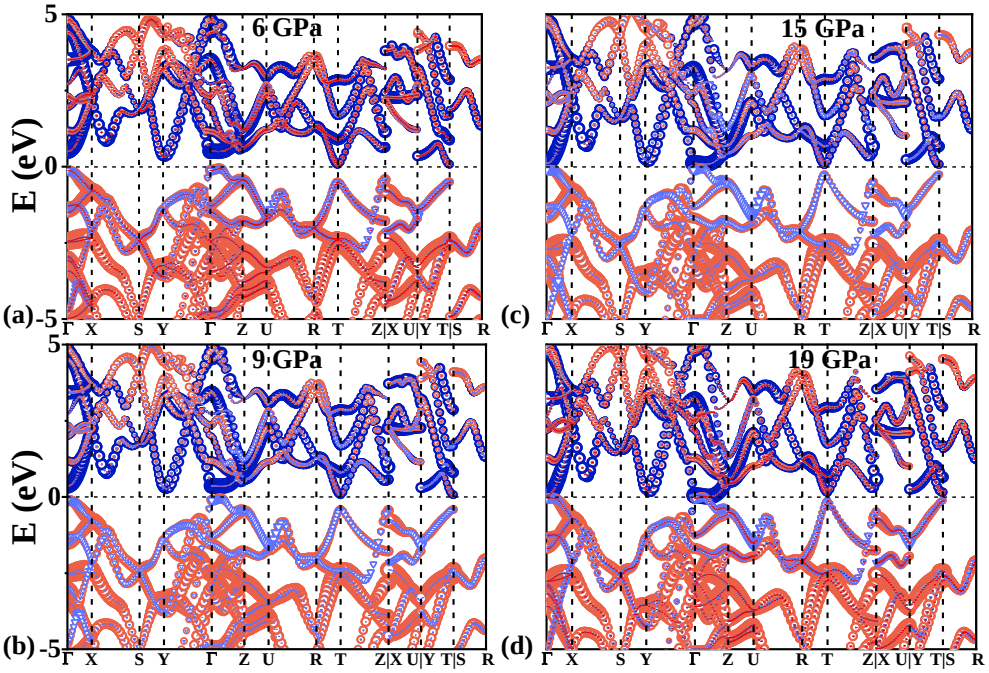

Fig. S5 Projected band structures of *Pnma*-2 GeS under different pressures. Red for S atoms, blue for Ge atoms, hollow circles for p orbitals, hollow inverted triangles for s orbitals, respectively. Since the contribution from the s-orbital of Ge atoms at VB near the Fermi surface (blue inverted triangles) would be completely obscured by the p-orbital of S atoms (red hollow circles), in order to better observe the variation of the contribution from the s-orbital of Ge atoms, we drew it in the upper layer.

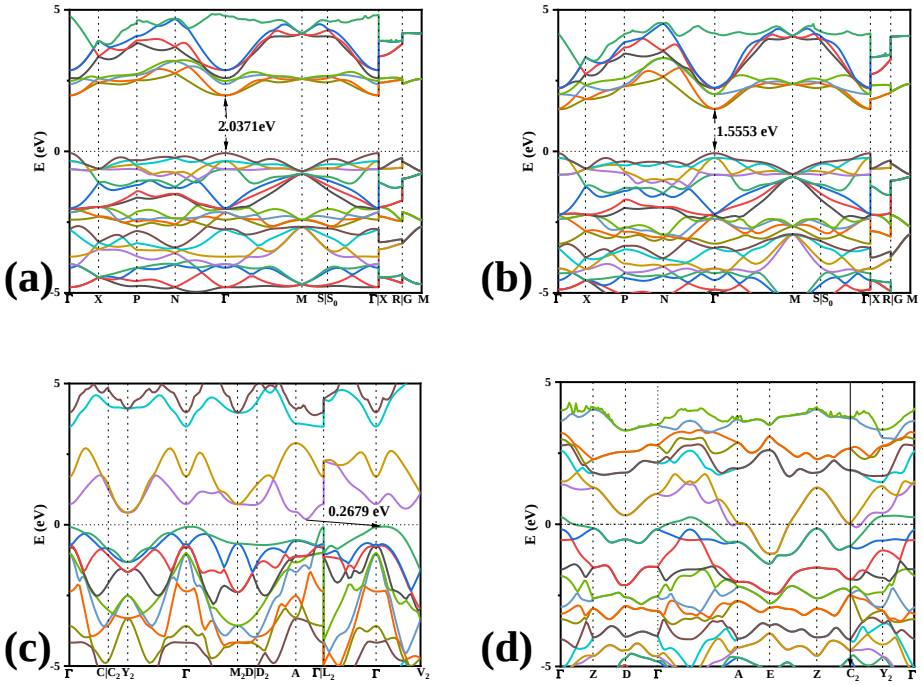

Fig. S6 Band structures of GeS_2 and GeS_4 under different pressures. Shown as, *I*-42*d* GeS_2 under 0 GPa (a) and 2.8 GPa (b), *C*2/*m* GeS_4 under 2.8 GPa (c), and $P2_1/c$ GeS_4 under 0 GPa.

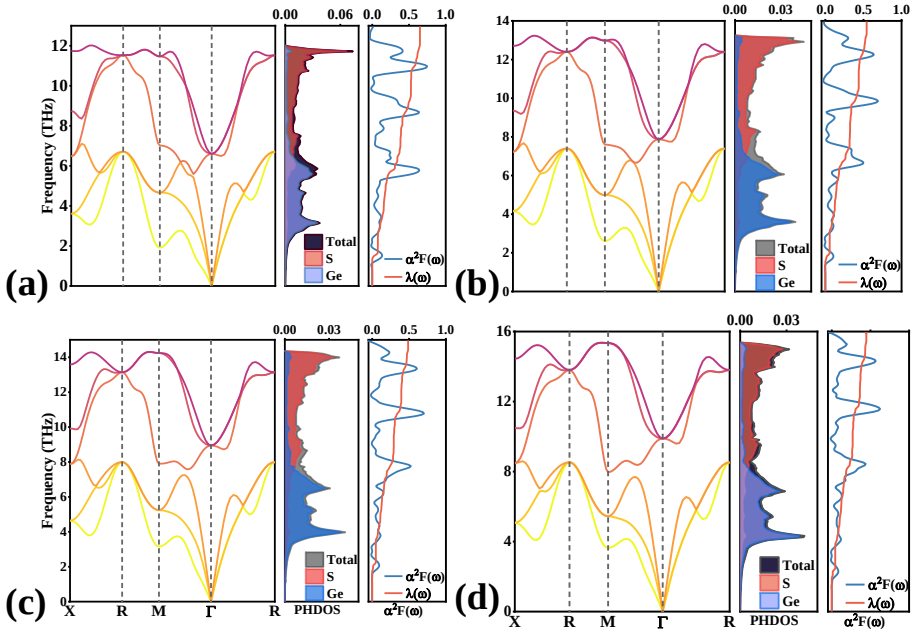

Fig. S7 Phonon, PDOS, λ and α²F(*ω*) for *Pm*-3*m* GeS at (a) 60 GPa, (b) 80 GPa, (c) 100 GPa and (d) 120 GPa.

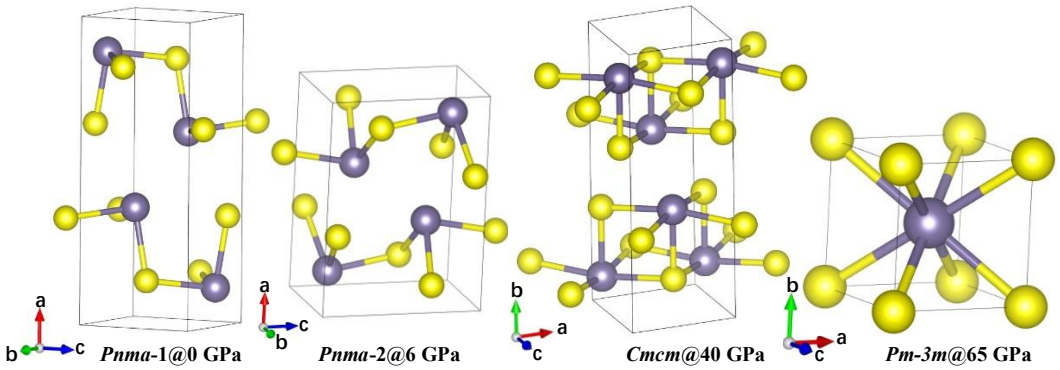

Fig. S8-A Crystal structures of GeS

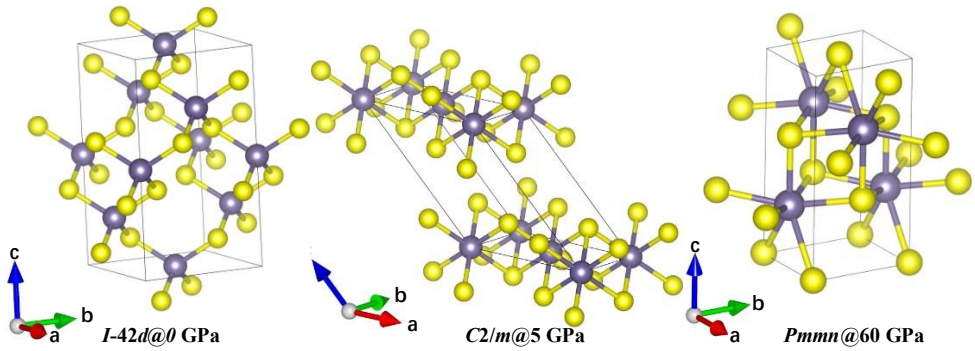

Fig. S8-B Crystal structures of GeS_2

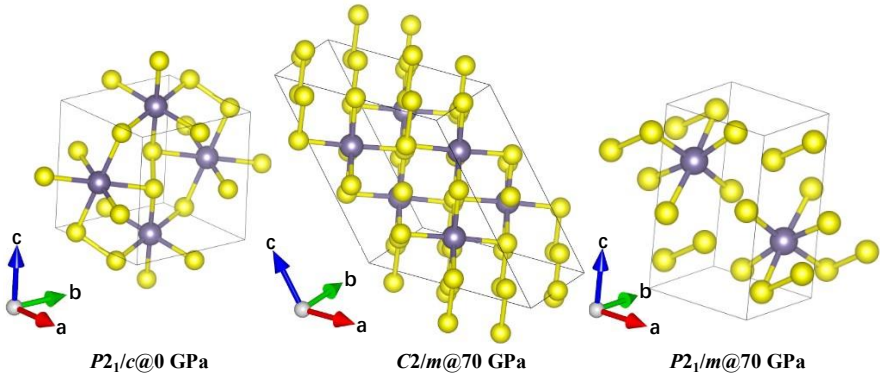

Fig S8-C Crystal structures of GeS_4