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Supporting Information

# Pressure-induced Changes in Crystal Structure and Electrical Conductivity of $GeV_4S_8$

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Table S1: Crystallographic data of the starting cubic and high-pressure orthorhombic phases of $GeV_4S_8$

| Space group | | |
|---|---|---|
| Pressure | ambient | 59.8 GPa |
| a (Å)<br>b (Å)<br>c (Å)<br>V (Å$^3$) | 9.6576<br><br><br>900.76 | 6.3577<br>6.7687<br>7.2481<br>311.910 |
| Atomic coordinates | Ga(1): 4a [0, 0, 0]<br>V(1):16e [0.60576, 0.60576, 0.60576]<br>S(1):16e [0.37049, 0.37049, 0.37049]<br>S(2):16e [0.86100, 0.86100, 0.86100] | Ga(1):2a [0, 0, 0]<br>V(1):4d [0, 0.21190, 0.64538]<br>V(2):4c [0.20805, 0, 0.44341]<br>S(1):4d [0, 0.75879, 0.36694]<br>S(11):4c [0.26053, 0, 0.75607]<br>S(2):4d [0, 0.70001, 0.95447]<br>S(21):4c [0.29172, 0, 0.14977] |

Table S2: Raman Band, band frequency, $\boldsymbol{\omega_o}$, at ambient condition, and Grneisen parameter, $\boldsymbol{\gamma}$, of the cubic phase of $GeV_4S_8$. The uncertainties are enclosed in the parenthesis.

| Region | Band | $\omega_o\ (cm^{-1})$ | $\frac{d\omega}{dP}\ (\frac{cm^{-1}}{GPa})$ | $\gamma$ |
|---|---|---|---|---|
| I | $A_1$ | 279.1(3.3) | 5.4(0.5) | 2.05(0.28) |
| | E | 414.2(1.7) | 4.4(0.2) | 1.12(0.11) |
| | E | 370.7(3.2) | 7.1(0.5) | 2.01(0.23) |
| | $B_1$ | 346.2(1.5) | 4.4(0.2) | 1.33(0.12) |
| II | $A_1$ | 318.5(1.7) | 2.1(0.1) | 0.68(0.05) |
| | E | 440.2(1.6) | 2.2(0.1) | 0.53(0.03) |
| | E | 418.0(4.1) | 3.6(0.1) | 0.90(0.08) |
| | $B_1$ | 370.7(1.7) | 2.4(0.1) | 0.69(0.04) |

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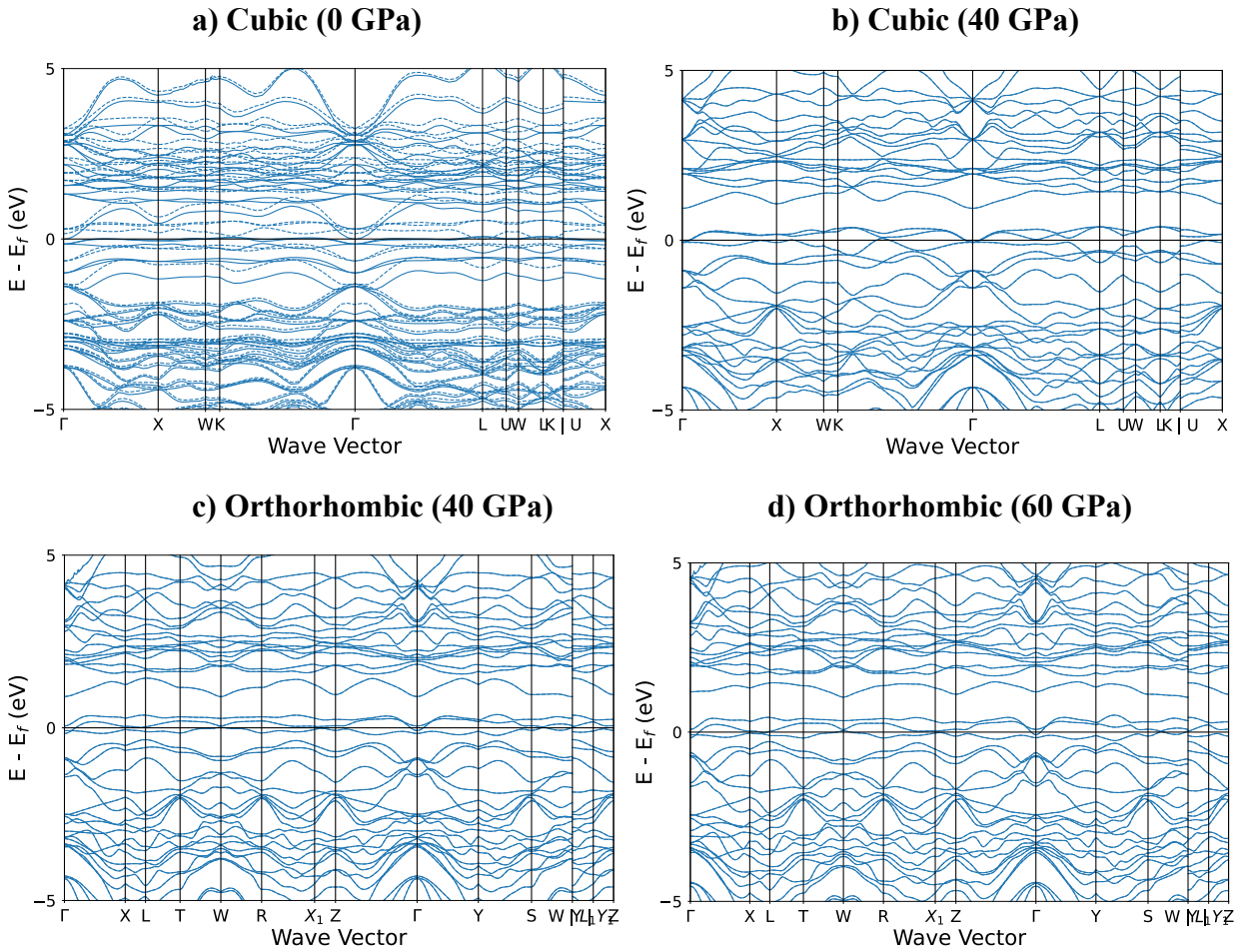


**Figure S1:** Electronic Band Structure for $GeV_4S_8$ calculated using GGA in primitive unit cell. The solid line represents spin up whereas dotted lines represent spin down.

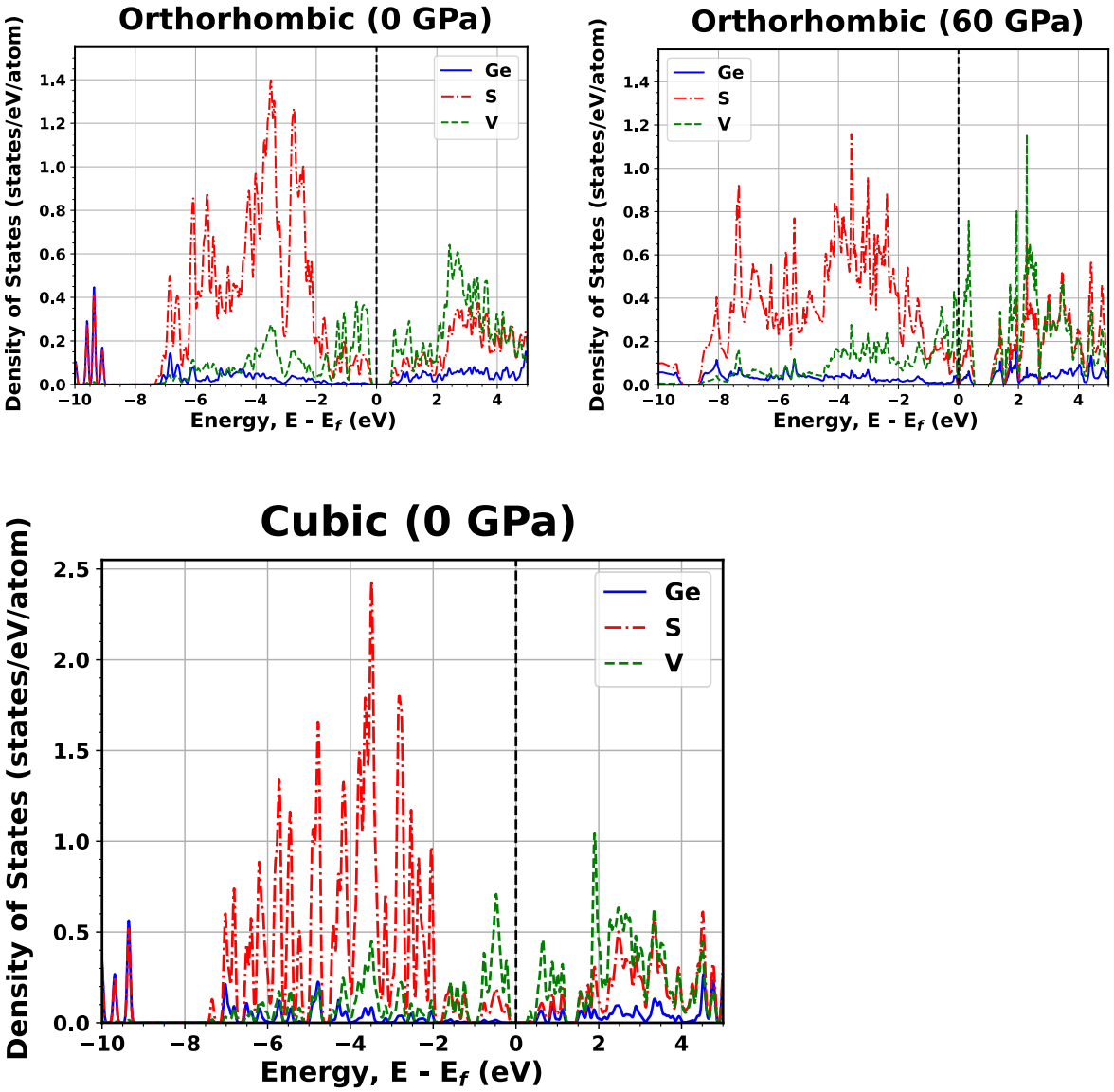


**Figure S2.** Electronic Local Density of States (LDOS) for $GeV_4S_8$ calculated using HSE06 in primitive unit cell at different pressures.