Supplementary Materials

Orientated hydrogen chains favor superconductivity in germanium sulfur hydrides

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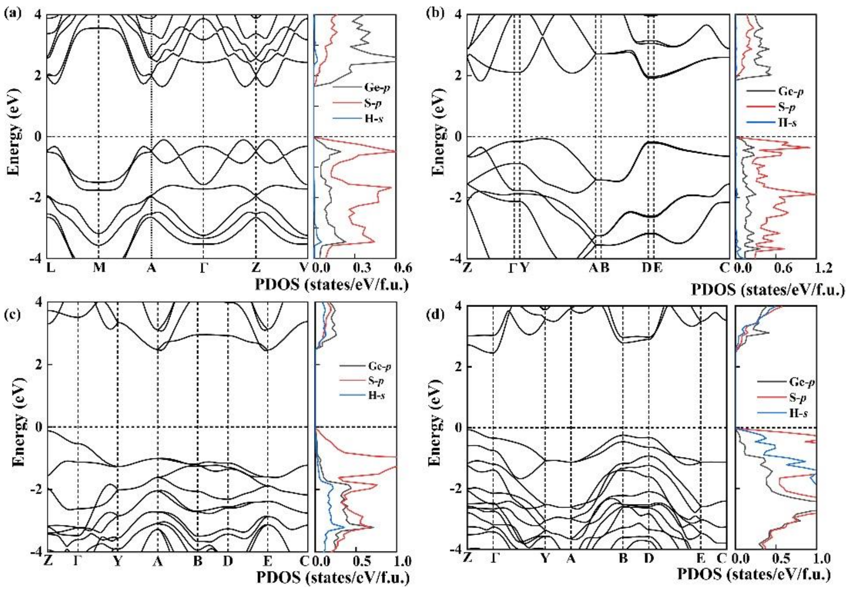

FIG. S1 Calculated electronic band structures and partial density of states (PDOS). (a) $C2$ $GeSH_{12}$ at 0 GPa, (b) $C2/c$ $GeSH_{14}$ at 0 GPa, (c) $P2_1$ $GeSH_{14}$ at 20 GPa and (d) $P2_1$ $GeSH_{16}$ at 20 GPa.

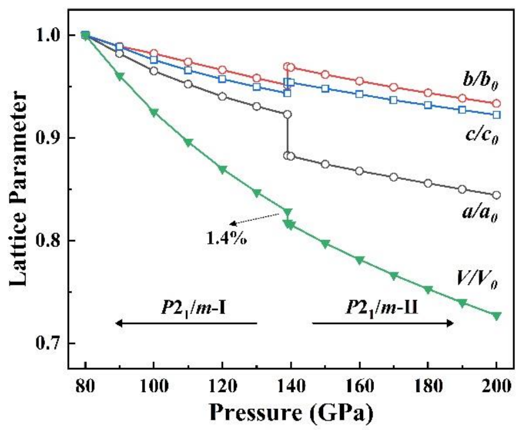

FIG. S2 The change of lattice parameters for $P2_1/m$ $GeSH_{14}$ with respect to pressure.

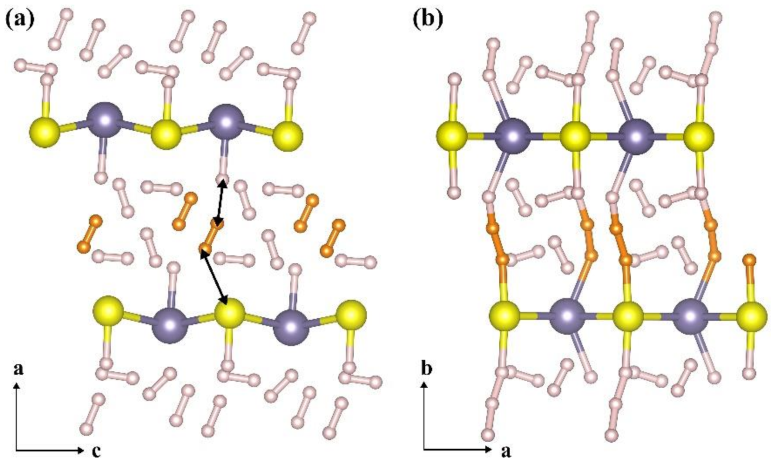

FIG. S3 The optimized crystal structures of (a) $P2_1/m$-I and (b) $P2_1/m$-II $GeSH_{14}$ at 139 GPa.

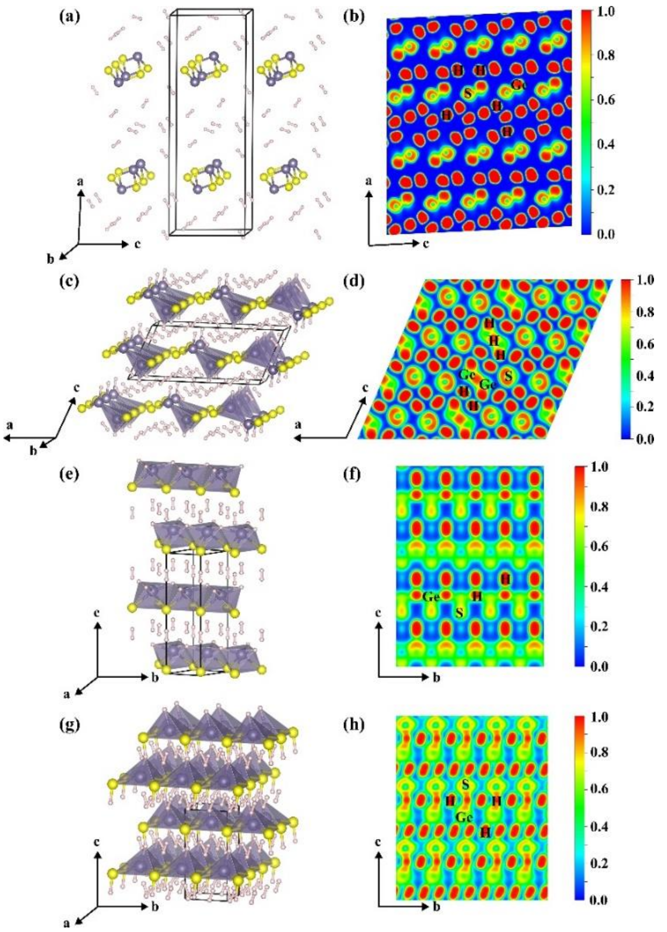

FIG. S4 The optimized crystal structures and corresponding valence electron localization function (ELF) for $GeSH_7$ at high pressure. (a) The *Cm* phase at 0 GPa and its ELF at (b). (c) The *C*2/*m* phase at 20 GPa and its ELF at (d). (e) The $P6_3mc$ phase at 60 GPa and its ELF at (f). (g) The $Pmn2_1$ phase at 140 GPa and its ELF at (h). Purple, yellow and pink spheres represent Ge, S and H atoms, respectively.

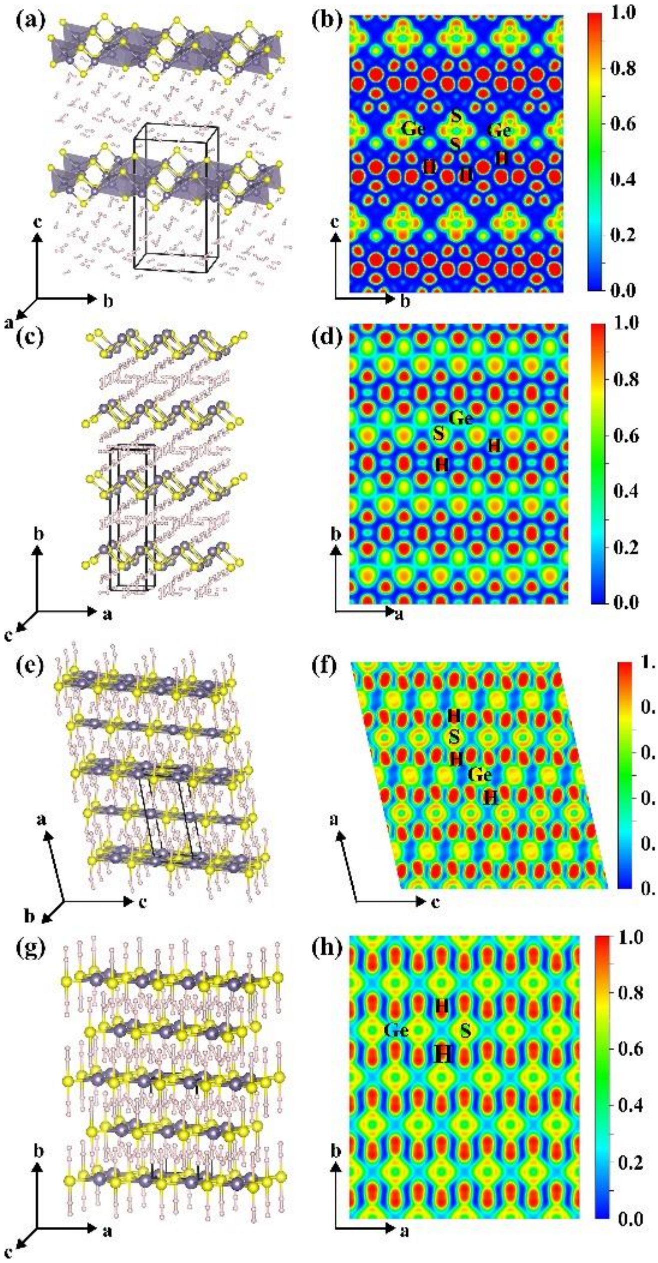

FIG. S5 The optimized crystal structures and corresponding valence electron localization function (ELF) for $GeSH_8$ at high pressure. (a) The *Cm* phase at 0 GPa and its ELF at (b). (c) The *Cmcm* phase at 20 GPa and its ELF at (d). (e) The *C*2/*m* phase at 80 GPa and its ELF at (f). (g) The *Cmmm* phase at 160 GPa and its ELF at (h). Purple, yellow and pink spheres represent Ge, S and H atoms, respectively.

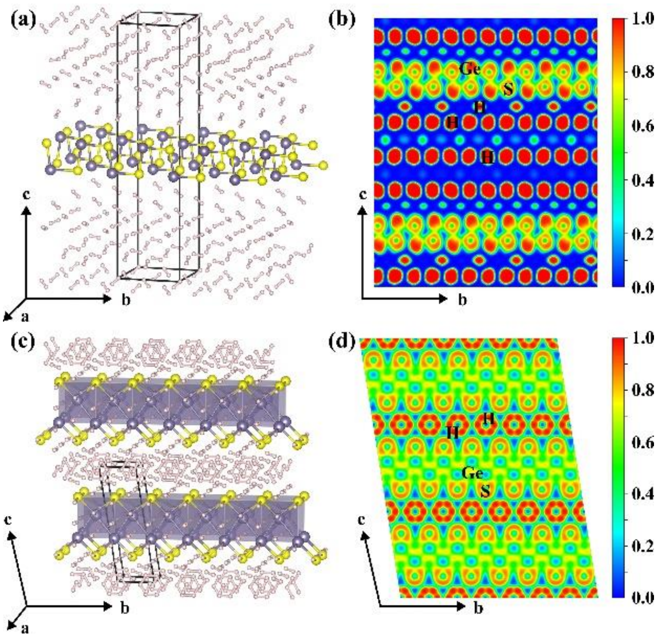

FIG. S6 The optimized crystal structures and corresponding valence electron localization function (ELF) for $GeSH_{12}$ at high pressure. (a) The *C*2 phase at 0 GPa and its ELF at (b). (c) The *P*-1 phase at 120 GPa and its ELF at (d). Purple, yellow and pink spheres represent Ge, S and H atoms, respectively.

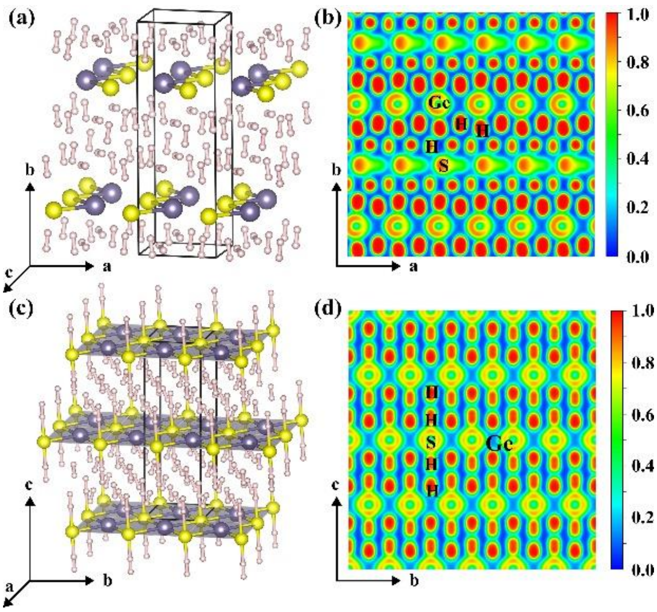

FIG. S7 The optimized crystal structures and corresponding valence electron localization function (ELF) for $GeSH_{16}$ at high pressure. (a) The $P2_1/m$ phase at 60 GPa and its ELF at (b). (c) The $P2_1/c$ phase at 100 GPa and its ELF at (d). Purple, yellow and pink spheres represent Ge, S and H atoms, respectively.

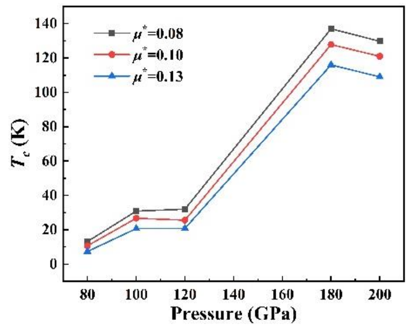

FIG. S8 The calculated T_c values of $P2_1/m$ $GeSH_{14}$ at various pressures by taking a series of μ^* = 0.08, 0.1 and 0.13.

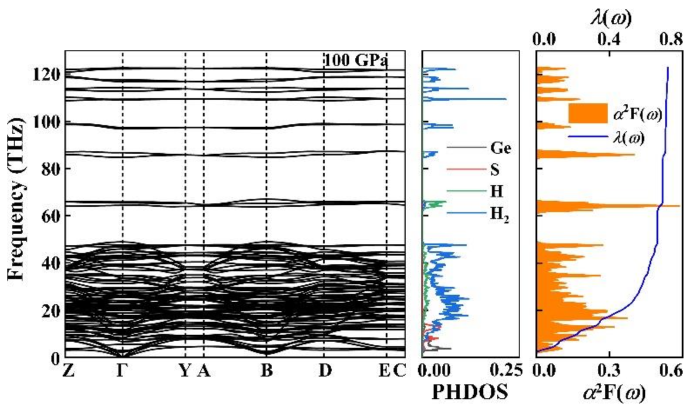

FIG. S9 The calculated phonon dispersions, phonon density of states (PHDOS), the Eliashberg spectral function $\alpha^2F(\omega)$ (orange area) and frequency-dependent electron–phonon coupling parameters $\lambda(\omega)$ (blue line) of $P2_1/m$-I $GeSH_{14}$ at 100 GPa.

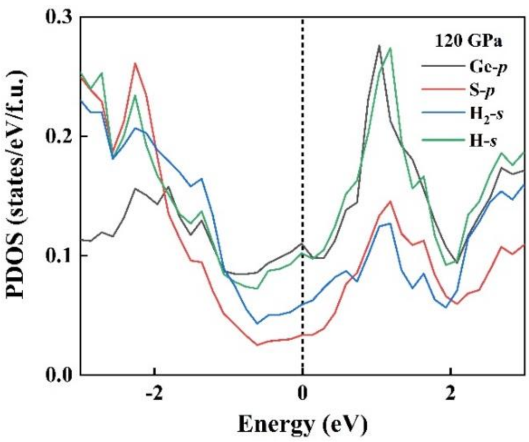

FIG. S10 Calculated partial density of states (PDOS) of $P2_1/m$-I $GeSH_{14}$ at 120 GPa

TABLE S1. Structural information of $P2_1/m$-I and $P2_1/m$-II phases of $GeSH_{14}$, $P2_1/m$ *and* $P2_1/c$ phases of $GeSH_{16}$.

Phase	Pressure (GPa)	Lattice parameters (Å, °)	Wyckoff positions (fractional)			
			Atom	x	y	z
$P2_1$ $GeSH_{14}$	20	*a*= 5.1173 *b*= 5.1618 *c*= 6.7489	Ge(2a)	0.6849	0.3557	0.5028
			S(2a)	0.2529	0.2801	0.5241
			H(2a)	-0.0097	0.5179	0.1383
			H(2a)	0.9372	0.9685	0.7738
			H(2a)	0.0640	0.1258	0.2065
			H(2a)	0.2419	0.2797	0.8738
			H(2a)	0.5317	0.5160	0.1451
			H(2a)	0.5904	0.9756	0.8026
			H(2a)	0.4782	0.5239	0.8438
			H(2a)	0.4109	0.1120	0.1814
			H(2a)	0.2936	0.8060	0.0360
			H(2a)	0.1951	0.7436	0.9717
			H(2a)	0.7889	0.2585	0.6985
			H(2a)	0.7672	0.2313	0.3089
			H(2a)	-0.0164	0.5105	0.8495
			H(2a)	0.7540	0.7951	0.0158
$P2_1/m$-I $GeSH_{14}$	80	*a*=10.8292 *b*= 3.1257 *c*= 3.4427	Ge(2e)	0.2335	0.2500	0.2876
			S(2e)	0.7428	0.2500	0.2266
			H(2e)	0.9561	0.2500	0.8926
			H(2e)	0.9751	0.2500	0.3385
			H(2e)	0.4041	0.2500	0.9430
			H(2e)	0.0848	0.2500	0.7268
			H(2e)	0.5980	0.2500	0.8011
			H(2e)	0.5591	0.2500	0.3874
			H(2e)	0.4115	0.2500	0.7274
			H(2e)	0.9007	0.2500	0.7495
			H(2e)	0.0941	0.2500	0.9523
			H(2e)	0.5089	0.7500	0.6537
			H(2e)	0.1324	0.7500	0.7625
			H(2e)	0.4576	0.7500	0.0779
			H(2e)	0.9539	0.7500	0.6201
			H(2e)	0.6258	0.7500	0.6600
$P2_1/m$-II $GeSH_{14}$	140	*a*=3.2751 *b*=9.5446 *c*=3.0294	Ge(2e)	0.72342	0.2500	0.8298
			S(2e)	0.2175	0.2500	0.3305
			H(4f)	0.4879	0.0706	0.8611
			H(4f)	0.8834	0.9943	0.7360
			H(4f)	0.6185	0.0442	0.3279
			H(4f)	0.7358	0.5943	0.1735
			H(4f)	0.0829	0.5814	0.1569

			H(4f)	0.2762	0.6149	0.6478
			H(4f)	0.1970	0.4072	0.3449
			Ge(2e)	0.3792	0.7500	0.1715
			S(2e)	0.8025	0.7500	0.6737
			H(4f)	0.0101	0.3759	0.8317
			H(4f)	0.2638	0.9411	0.6664
$P2_1/m$ $GeSH_{16}$	60	*a*= 3.7985 *b*=11.2700 *c*= 3.2441	H(4f)	0.2427	0.6253	0.6572
			H(4f)	0.9946	0.0577	0.8467
			H(4f)	0.2263	0.4109	0.3273
			H(4f)	0.4301	0.4157	0.7380
			H(4f)	0.4755	0.5752	0.0607
			H(4f)	0.7521	0.9788	0.665
			Ge(2b)	0.5000	0.0000	1.0000
			S(2c)	0.0000	0.0000	0.5000
			H(4e)	0.9263	0.0012	0.8735
			H(4e)	0.3618	0.2234	0.7948
$P2_1/c$ $GeSH_{16}$	100	*a*= 3.0452 *b*= 3.5638 *c*=10.9695	H(4e)	0.8671	0.4993	0.7755
			H(4e)	0.3583	0.7754	0.7952
			H(4e)	0.5874	0.7950	0.6386
			H(4e)	0.1442	0.4980	0.6959
			H(4e)	0.4158	0.7037	0.8618
			H(4e)	0.8991	0.4995	0.8497
P-1 $GeSH_{12}$	100	*a*= 3.0452 *b*= 3.5638 *c*=10.9695				

TABLE S2. Superconducting properties of $GeSH_{16}$ under pressure. The μ^* value for the T_c calculation is 0.1.

Phase	Pressure (GPa)	λ	ω_{log} (K)	$N(E_f)$ (states/Ry)	T_c (K)
$P2_1/m$	60	0.58	333.6	6.9	5.3
	80	0.83	249.8	4.2	16.7
$P2_1/c$	140	1.41	596.5	14.0	63.7
	160	1.70	481.3	14.1	72.4
	180	2.23	317.0	13.8	62.1
	200	1.26	561.2	11.7	53.4