Supporting Information

Superconducting H_7 chain in gallium hydrides at high pressure

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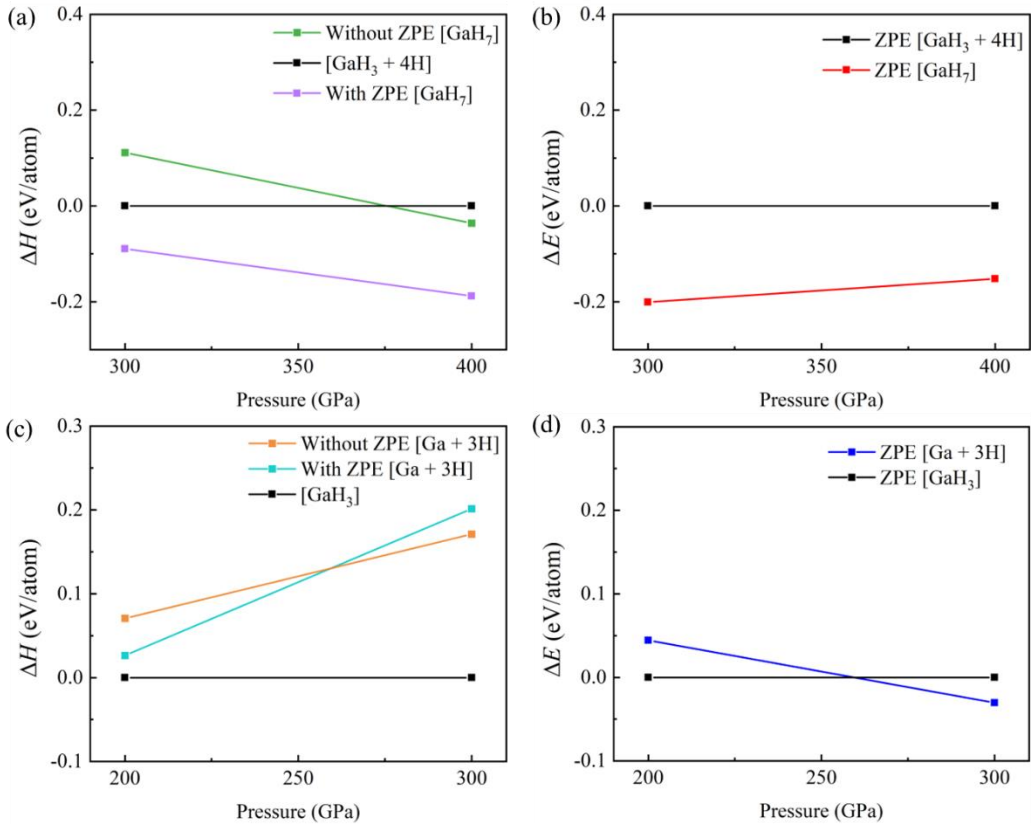

FIG. S1. Relative enthalpies of GaH_7 (a) and GaH_3 (c) with and without inclusion of ZPE as a function of pressure. (b) and (d) are the relative ZPE of GaH_7 and GaH_3 as a function of pressure, respectively.

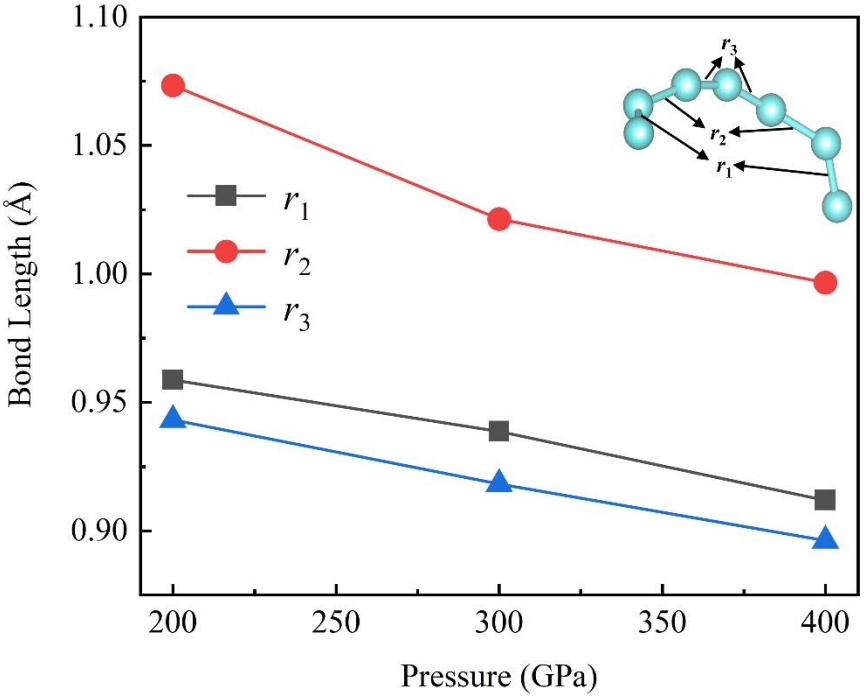

FIG. S2 bond length of Ga-H system at different pressures.

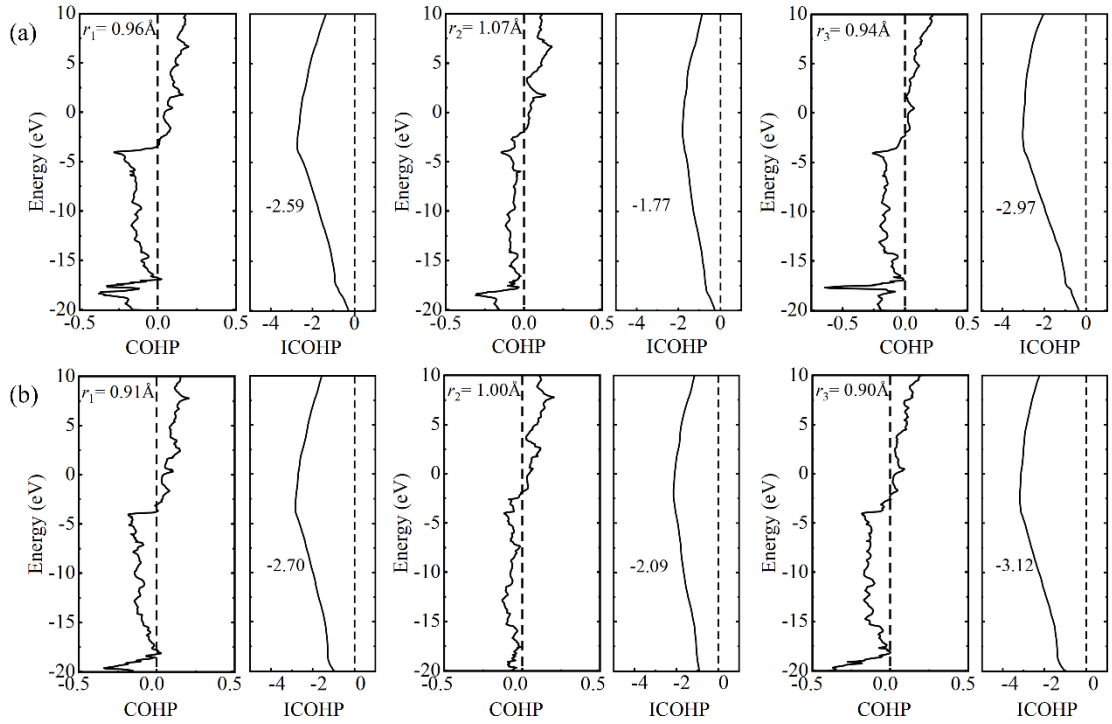

FIG. S3 The calculated crystalline orbital Hamiltonian population (COHP) and integrated crystalline orbital Hamiltonian population (ICOHP)of GaH_7 for three different H-H distances in H_7 chain at 200 GPa (a) and 400 GPa (b).

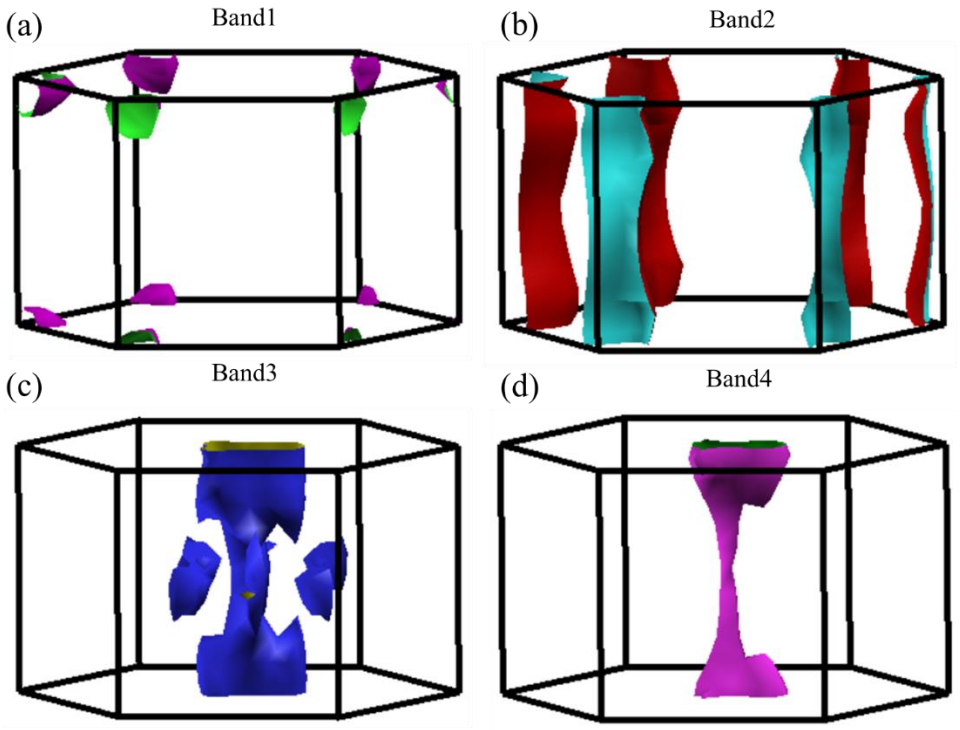

FIG. S4 The Fermi surfaces of GaH_7 associated with the four bands that contribute significantly to the electronic band structure at 300 GPa.

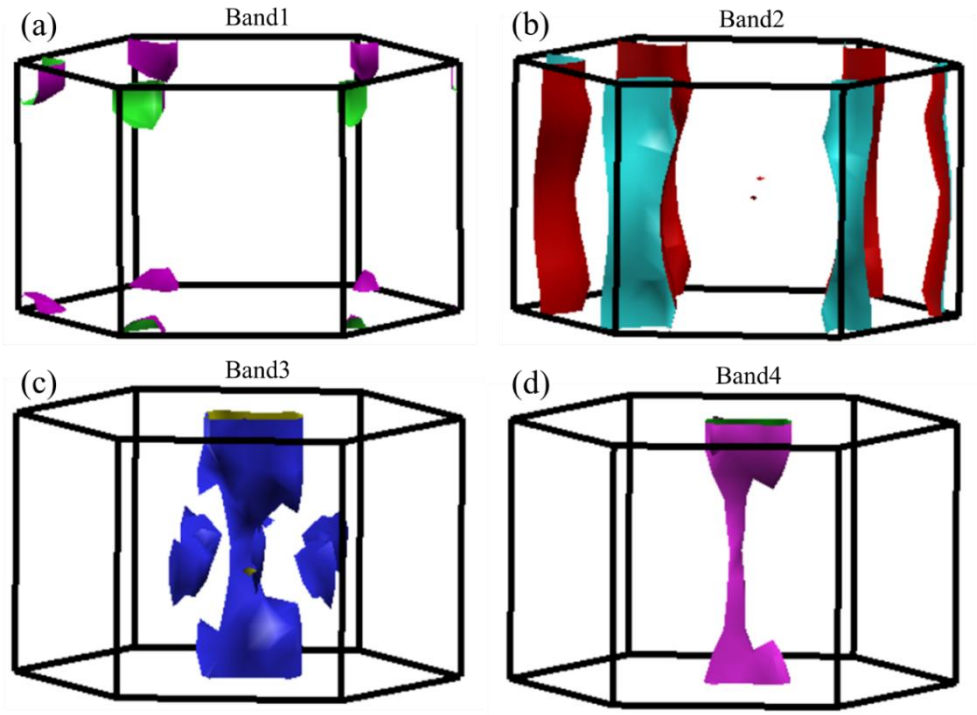

FIG. S5 The Fermi surfaces of GaH_7 associated with the four bands that contribute significantly to the electronic band structure at 200 GPa.

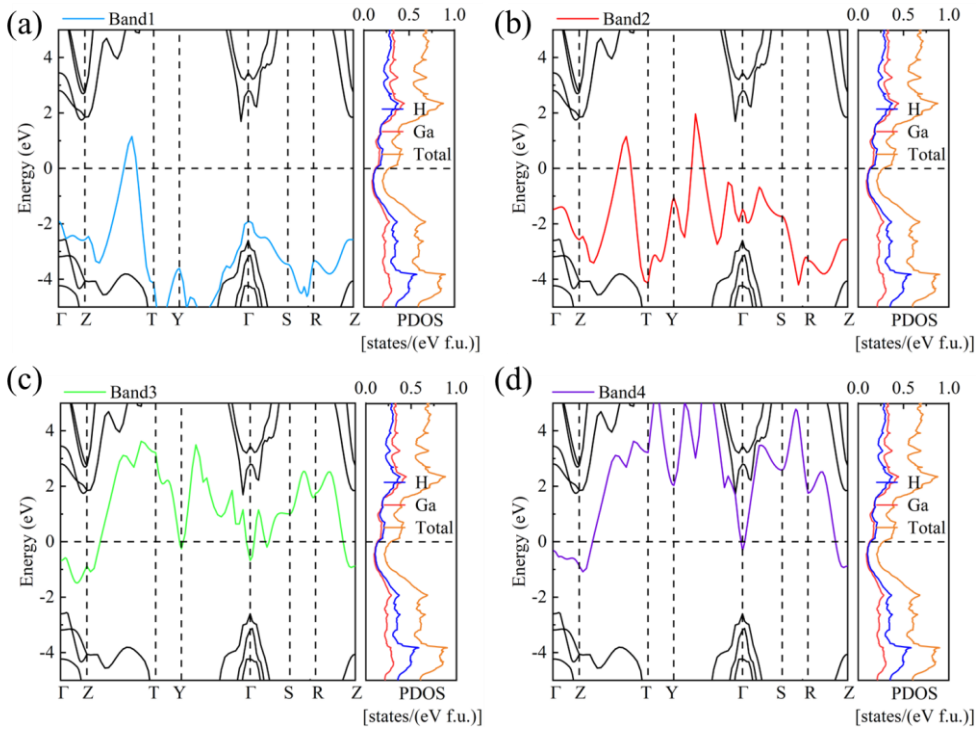

FIG. S6. The band structure and the density of states (DOS) of GaH_7 at 300GPa.

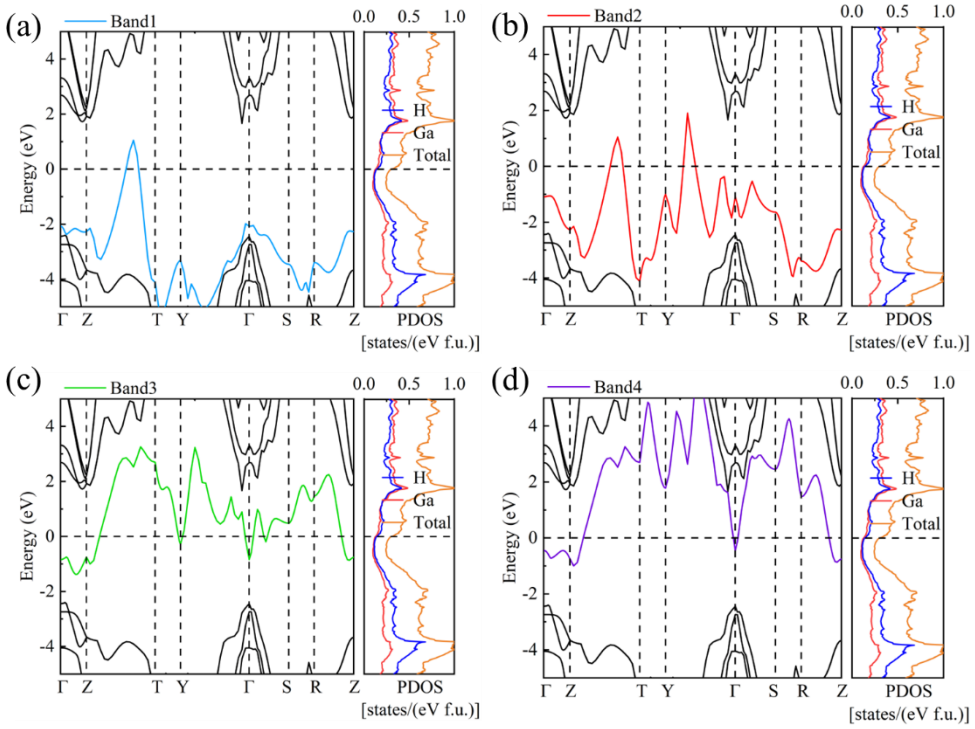

FIG. S7. The band structure and the density of states (DOS) of GaH_7 at 200GPa.

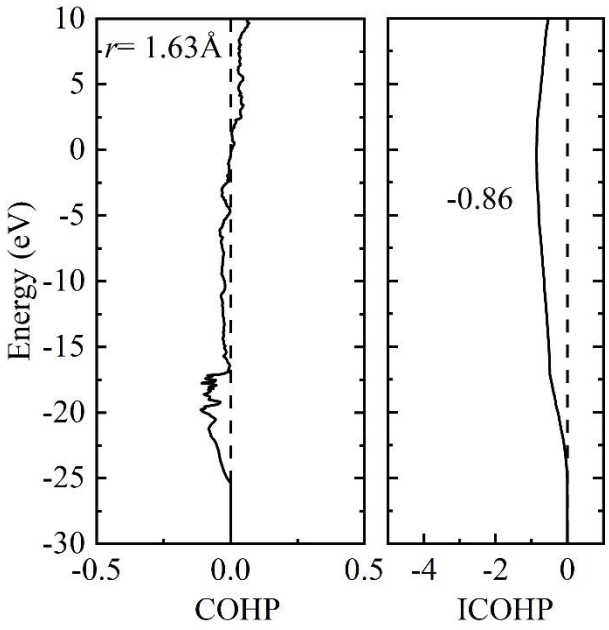

FIG. S8 The calculated crystalline orbital Hamiltonian population (COHP) and integrated crystalline orbital Hamiltonian population (ICOHP) of GaH_7 for the shortest Ga-H distances in GaH_7 at 300 GPa

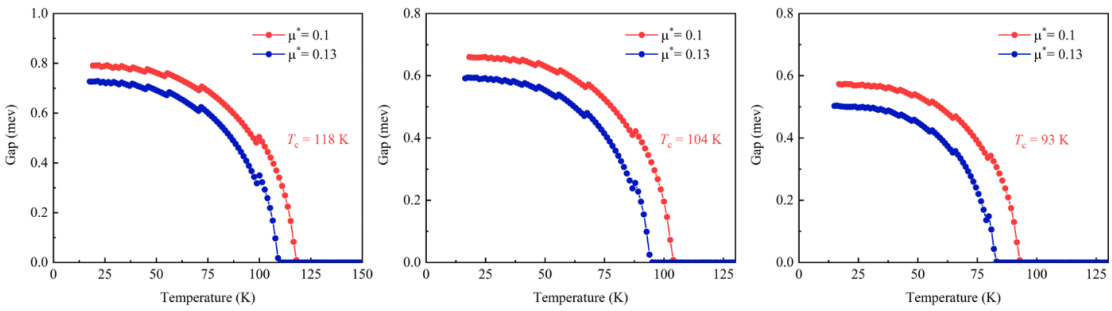

FIG. S9. Calculated anisotropic superconducting gap of GaH_7 at 200 GPa, 300 GPa and 400 GPa.

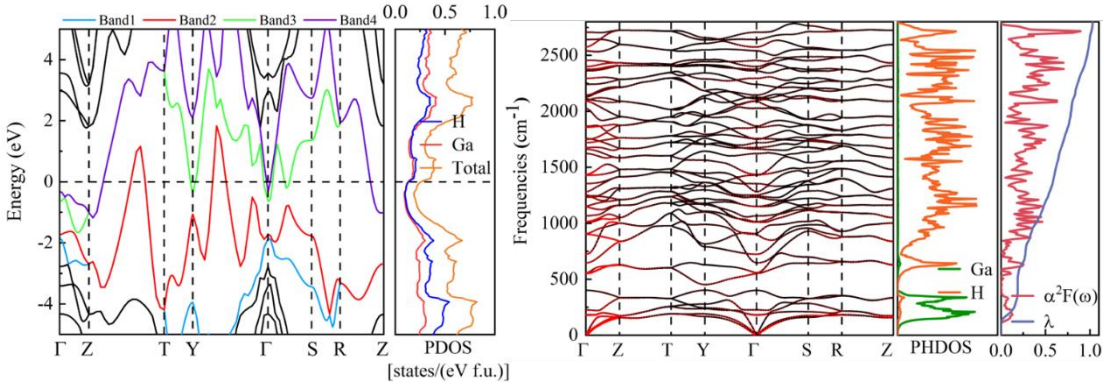

FIG. S10. Electronic band structure and projected density of states (PDOS), phonon-dispersion curves, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$ and the EPC parameter λ of GaH_7 at 400 GPa.

Table. S1. Charge transfer of Ga and H of $C222_1$ GaH_7 in one unit cell at different pressures. The negative and positive sign indicate electron gain and loss, respectively.

Pressure (GPa)	Atoms	Charge (e)
200	H1	–0.22
	H2	–0.15
	H3	–0.10
	H4	–0.12
	Ga	+1.06
300	H1	–0.24
	H2	–0.15
	H3	–0.10
	H4	–0.13
	Ga	+1.12
400	H1	–0.25
	H2	–0.15
	H3	–0.11
	H4	–0.13
	Ga	+1.16

Table. S2. Structural information of GaH_7.

Space group	Lattice parameter (Å, °)	atomic coordinate	*x*	*y*	*z*	sites
$C222_1$	*a*=5.460	H1	-0.077	0.699	1.123	8*c*
	b= 3.142	H2	-0.209	0.524	1.180	8*c*
(300 GPa)	*c*= 4.193	H3	-0.212	0.771	1.435	8*c*
	α=β=γ=90	H4	0.174	0.500	1.000	4*a*
		Ga	0.000	0.835	0.750	4*b*

Table. S3. The calculated electron-phonon coupling parameter (λ), logarithmic average phonon frequency (ω_{log}), and the estimated T_c for GaH_7 using the Allen-Dynes modified McMillan (ADM) equation, and numerically solving the Eliashberg equations with $\mu^* = 0.1$.

			T_c (K)	
Pressure (GPa)	λ	ω_{log} (K)	ADM	Eliashberg
200	1.35	902	93	118
300	1.01	1291	91	104
400	0.89	1431	82	93