Supporting Information:

First-Principles Investigation of the Phase Diagram and Superconducting Properties of the Sc-Mg-H System under High Pressure

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Table S1. Crystallographic data of the newly predicted structures of ternary Sc-Mg-H compounds under high pressure (P, in GPa). The unit of lattice parameters (*a*, *b*, and *c*) is given in Å.

Compound	Space group	P (GPa)	Lattice parameters (Å,°)	Atomic coordinates (fractional)			
				Atoms	*x*	*y*	*z*
$ScMgH_6$	*P4/mmm*	100	$a = b = 2.8422$	Sc(1b)	0.0000	0.0000	0.5000
			$c = 4.08845$	Mg(1c)	0.5000	0.5000	0.0000
			$\alpha = \beta = \gamma = 90$	H(4i)	0.0000	0.5000	0.2379
				H(1a)	0.0000	0.0000	0.0000
				H(1d)	0.5000	0.5000	0.5000
$ScMgH_8$	*P4/mmm*	80	$a = 5.08074$	Sc(1a)	0.0000	0.0000	0.0000
			$b = 3.45602$	Mg(1d)	0.5000	0.5000	0.5000
			$c = 4.92299$	H(4i)	0.0000	0.5000	0.2586
			$\alpha = \beta = \gamma = 90$	H(2g)	0.0000	0.0000	0.4070
				H(2h)	0.5000	0.5000	0.0956
$ScMgH_{12}$	*Cmmm*	100	$a = b$=3.07238	Sc(1d)	0.0000	0.0000	0.5000
			$c = 4.92299$	Mg(1b)	0.5000	0.0000	0.0000
			$\alpha = \beta = \gamma = 90$	H(4o)	0.3818	0.0000	0.3743
				H(4m)	0.2500	0.2500	0.2253
				H(4o)	0.1276	0.0000	0.1304
Sc_2MgH_{18}	$P\bar{3}m1$	150	$a = b = 4.8195$	Sc(2d)	0.3333	0.6667	0.6587
			$c = 2.92736$	Mg(1a)	0.0000	0.0000	0.0000
			$\alpha = \beta = 90$	H(12j)	0.9170	0.5882	0.8404
			$\gamma = 120$	H(6h)	0.2425	0.0000	0.5000
$ScMg_2H_{18}$	$P\bar{3}m1$	200	$a = b = 4.6217$	Sc(1b)	0.0000	0.0000	0.5000
			$c = 2.83856$	Mg(2d)	0.3333	0.6667	0.1693
			$\alpha = \beta = 90$	H(12j)	0.5785	0.9140	0.6703
			$\gamma = 120$	H(6g)	0.2617	0.0000	0.0000

Table S2. Calculated elastic constants C_{ij} and bulk (B), shear (G), Young's (Y) moduli and Poisson's ratio (σ) of the stable phase of Sc–Mg–H systems selected pressures.

	$ScMgH_8$	$ScMgH_{12}$	Sc_2MgH_{18}	$ScMg_2H_{18}$
	100 GPa	100 GPa	260 GPa	150 GPa
C_{11}	578.64	524.41	3718.84	768.73
C_{12}	70.80	225.22	401.58	383.00
C_{13}	209.90	206.63	531.24	309.61
C_{14}	0.00	0.00	-33.85	12.73
C_{22}	0.00	450.25	0.00	0.00
C_{23}	0.00	216.35	0.00	0.00
C_{33}	594.05	516.22	671.28	0.00
C_{44}	161.16	126.93	261.94	201.52
C_{55}	0.00	133.43	0.00	0.00
C_{66}	71.64	153.65	158.63	192.86
B	300.95	309.20	557.46	478.91
G	150.05	138.27	154.33	205.17
B/G	2.01	2.24	3.61	2.33
Y	386.01	361.00	423.88	538.60
σ	0.29	0.31	0.37	0.31

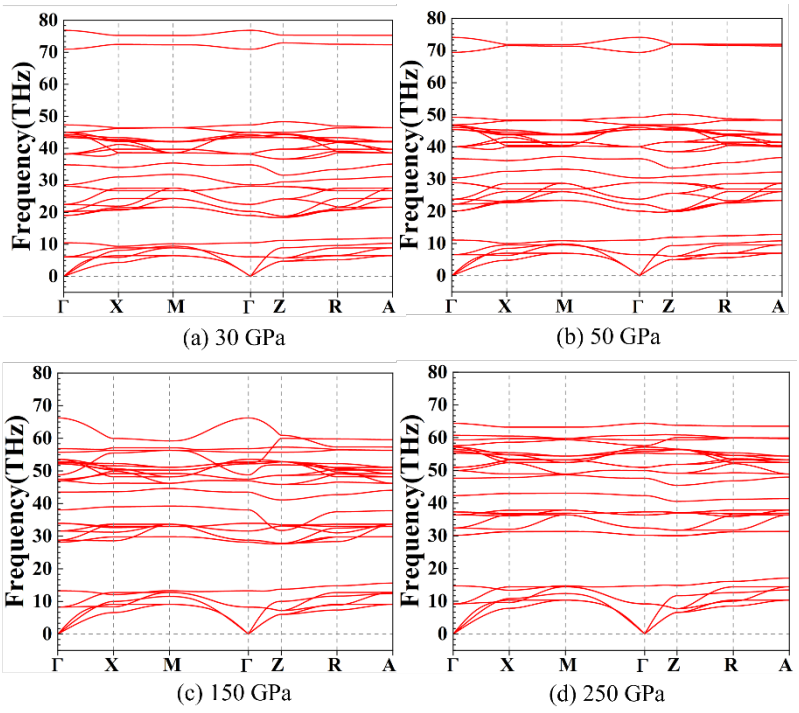

Fig. S1. Pressure-dependent phonons and electron-phonon coupling spectra for $ScMgH_8$.

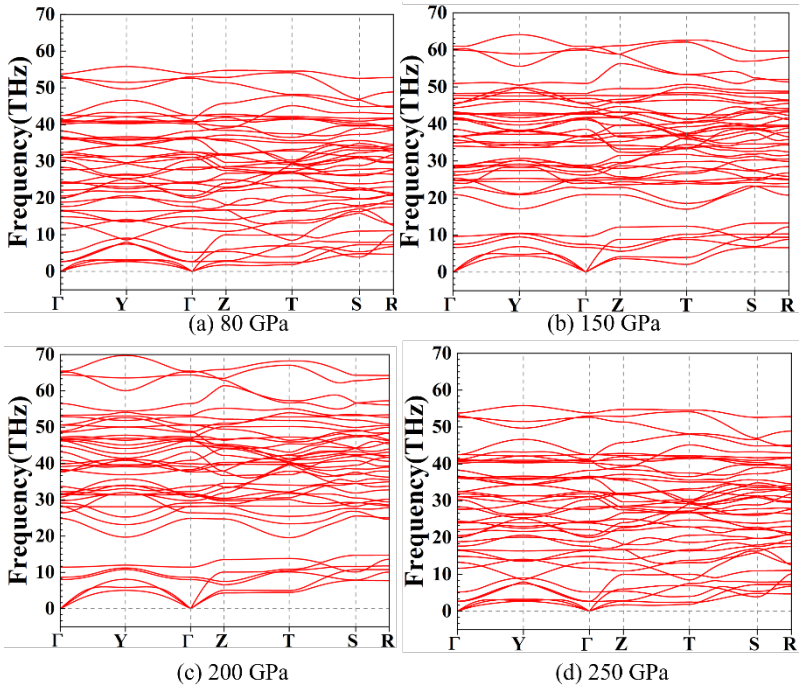

Fig. S2. Pressure-dependent phonons and electron-phonon coupling spectra for $ScMgH_{12}$.

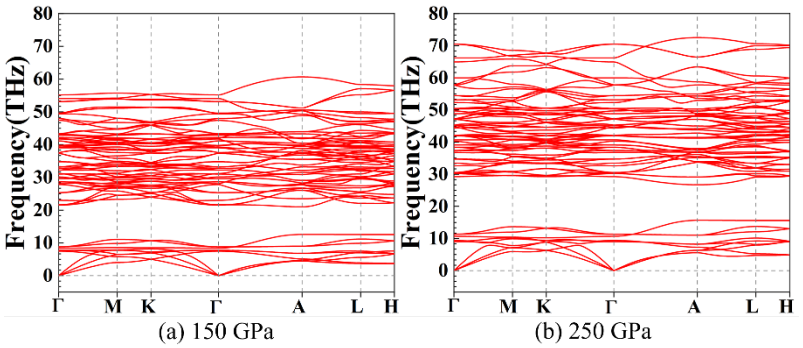

Fig. S3. Pressure-dependent phonons and electron-phonon coupling spectra for Sc_2MgH_{18}.

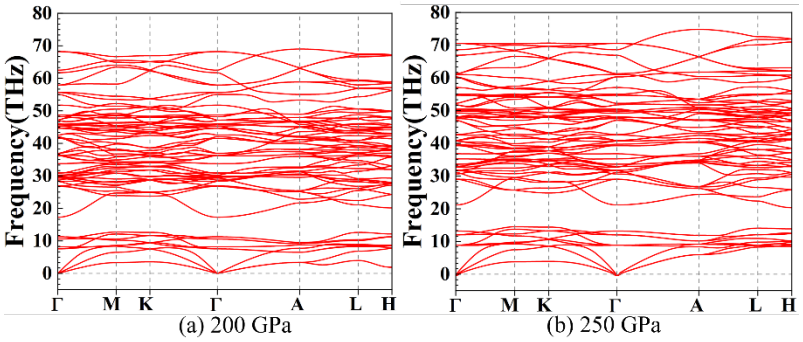

Fig. S4. Pressure-dependent phonons and electron-phonon coupling spectra for $ScMg_2H_{18}$.

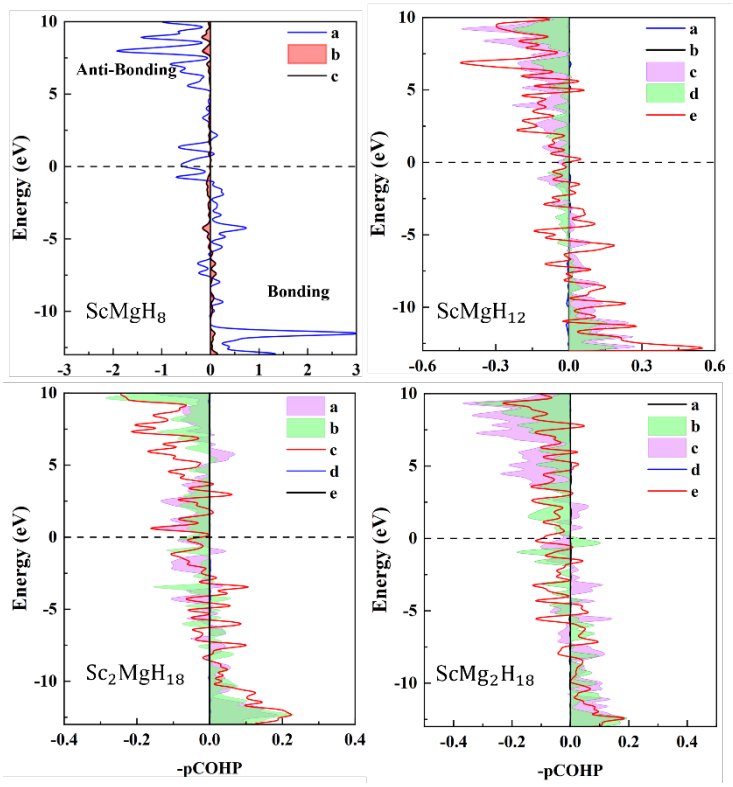

Fig. S5 The -pCOHP for pairs of H...H of (a) $ScMgH_8$, (b) $ScMgH_{12}$, (c) Sc_2MgH_{18}, and (d) $ScMg_2H_{18}$.

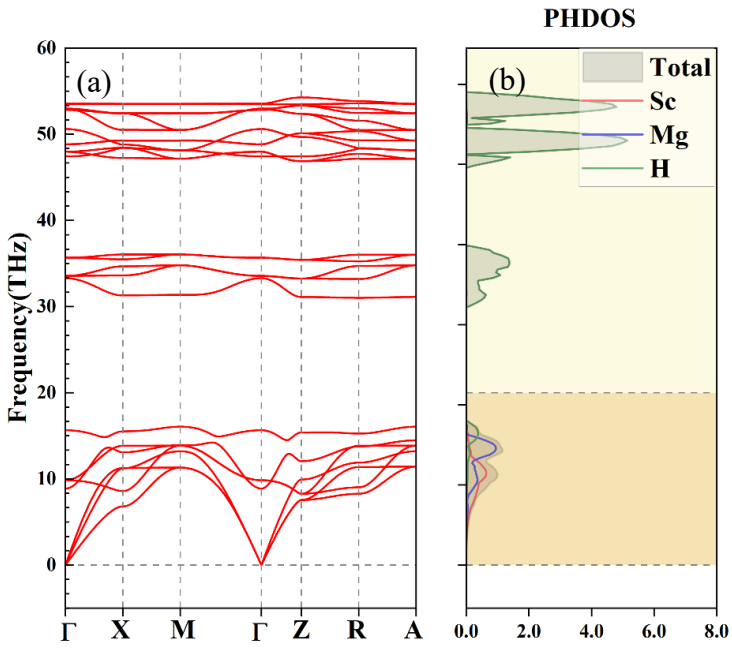

Fig. S6. (a) Phonons and (b) PHDOS for $ScMgH_6$ at 100 GPa.

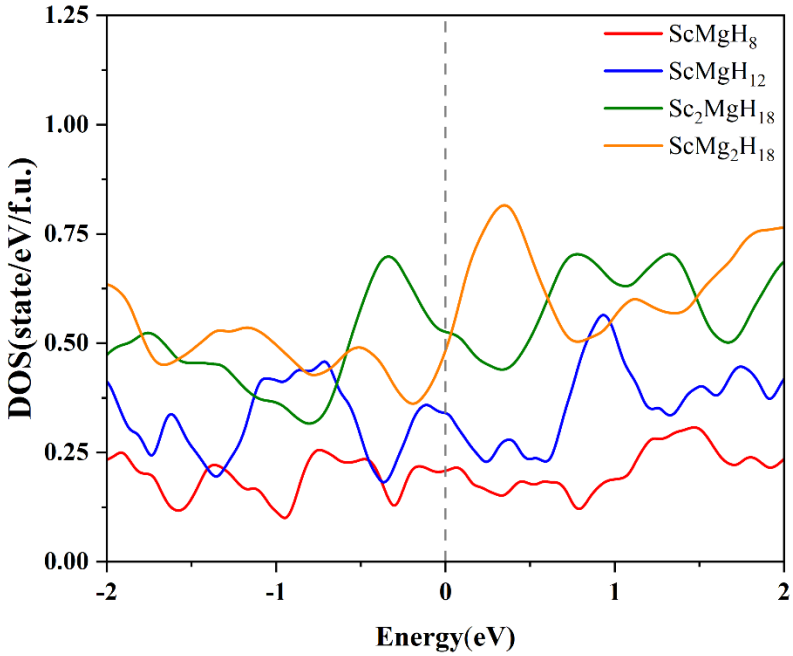

Fig. S7. Partial DOS of H atoms in $ScMgH_8$, $ScMgH_{12}$, Sc_2MgH_{18}, and $ScMg_2H_{18}$.

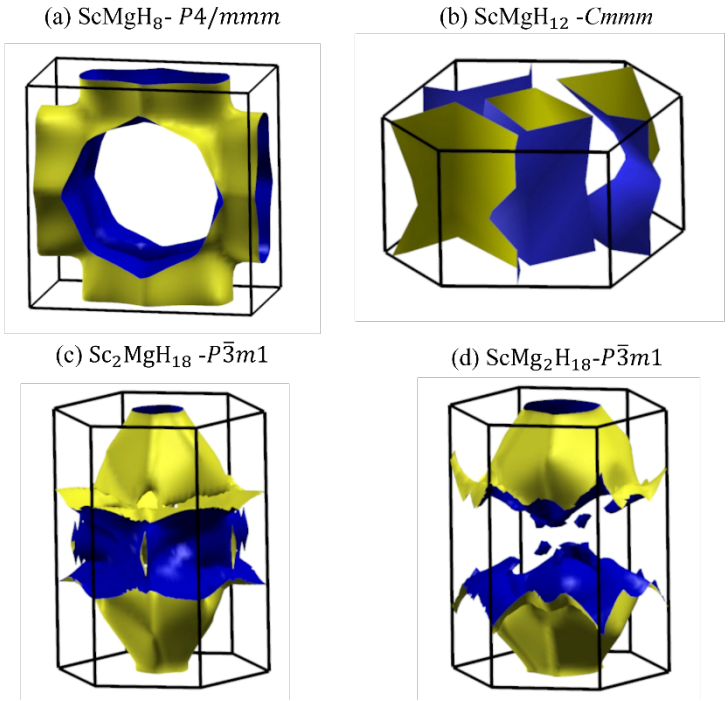

Figure S8. The Fermi surface of (a) $ScMgH_8$- *P*4/*mmm* at 80 GPa, (b) $ScMgH_{12}$ -*Cmmm* at 100 GPa, (c) Sc_2MgH_{18} -$P\bar{3}m1$ at 150 GPa, and (d) $ScMg_2H_{18}$ - $P\bar{3}m1$ at 200 GPa.