Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Prediction of superconducting ternary hydride $MgGeH_6$: from divergent high-pressure formation routes

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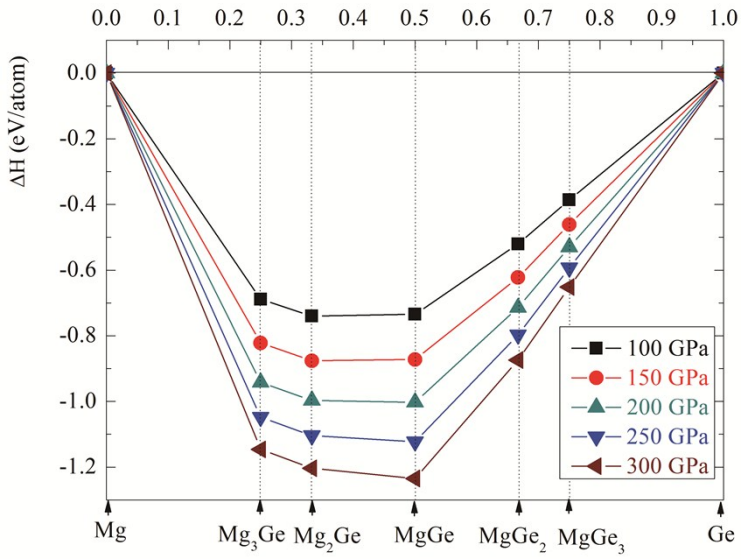

Fig. S1 The formation enthalpies of Mg-Ge with respect to decomposition into Mg and Ge at selected pressures.

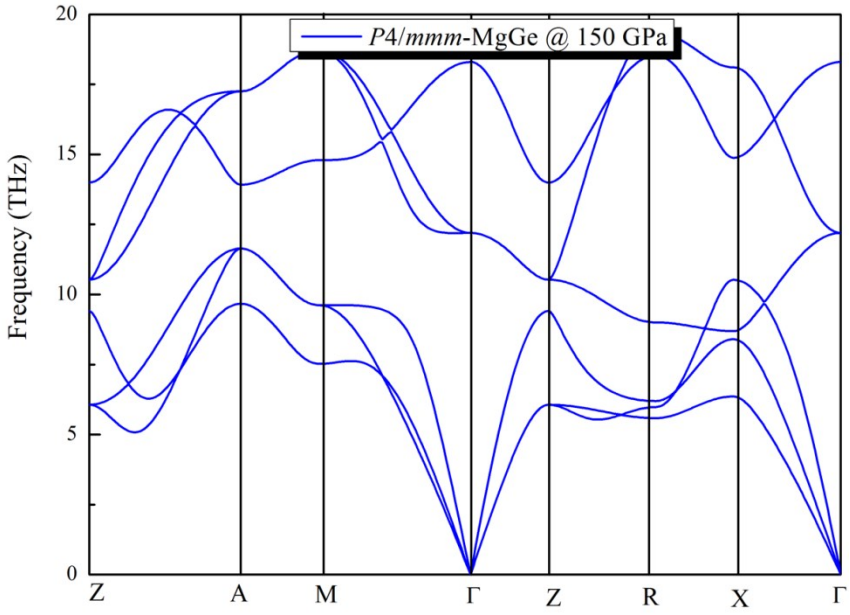

Fig. S2 Phonon band structures of *P*4/*mmm* MgSi at 150 GPa. No any imaginary frequency modes demonstrate that it is dynamically stable.

Table S1 Elastic constants C_{ij} (GPa) of *P*4/*mmm*-MgGe at 150 GPa.

MgGe	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
(150 GPa)	668.90	209.10	291.14	619.60	215.81	96.32

For tetragonal MgGe, the mechanical stability criteria are given by $C_{11}>0$, $C_{33}>0$, $C_{44}>0$, $C_{66}>0$, $(C_{11}-C_{12})>0$, $(C_{11}+C_{33}-2C_{13})>0$ and $[2(C_{11}+C_{12})+C_{33}+4C_{13}]>0$.

Obviously, elastic constants satisfy mechanical stability criteria, demonstrating *P*4/*mmm*-MgGe is mechanically stable at 150 GPa.

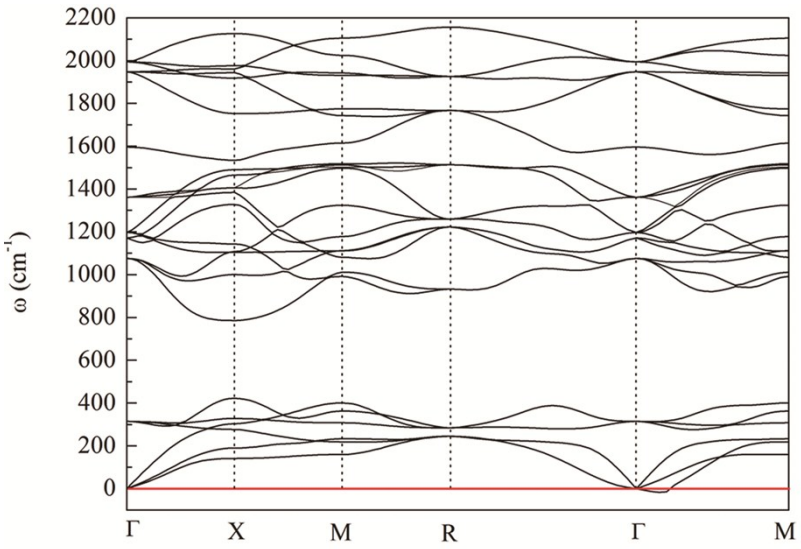

Fig. S3 The phonon band structure of $MgGeH_6$ at 150 GPa. Imaginary frequency around Γ point demonstrates that it is dynamically unstable.