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 $P4/mmm$ MgSi at 150 GPa. No any imaginary frequency modes demonstrate that it is dynamically stable.
Table S1 Elastic constants $C_{ij}$ (GPa) of $P4/mmm$-MgGe at 150 GPa.

<table>
<thead>
<tr>
<th>MgGe</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{13}$</th>
<th>$C_{33}$</th>
<th>$C_{44}$</th>
<th>$C_{66}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(150 GPa)</td>
<td>668.90</td>
<td>209.10</td>
<td>291.14</td>
<td>619.60</td>
<td>215.81</td>
<td>96.32</td>
</tr>
</tbody>
</table>

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 $P4/mmm$-MgGe is mechanically stable at 150 GPa.

Fig. S3 The phonon band structure of MgGeH$_6$ at 150 GPa. Imaginary frequency around $\Gamma$ point demonstrates that it is dynamically unstable.