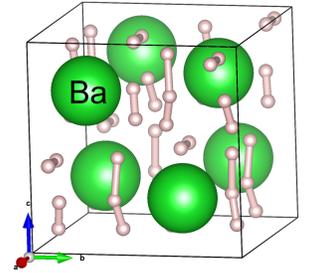


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Overview

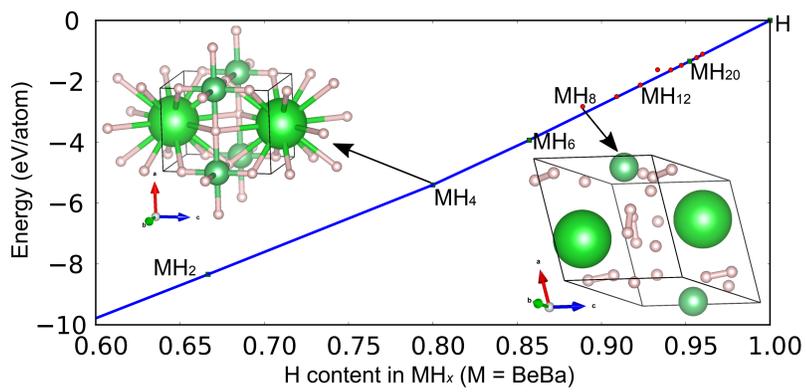
Chen et al. [Nat Commun 12, 273 (2021)] reported the superconducting temperature T_S of 20 K in the synthesized BaH_{12} at 140 GPa. In order to break the molecular units and improve the T_S at the moderate pressures, we introduce light elements into the barium superhydrides. Herein, we use high-throughput crystal structure prediction methods by combing CALYPSO, CrySPY with VASP to screen the low-lying structures of $BeBaH_x$ ($x = 1$ to 24) at pressures up to 100 GPa. By screening over 100,000 crystal structures, we obtain the phase diagram of $BeBaH_x$. In addition, $BeBaH_4$ and $BeBaH_8$ are found to be dynamically stable at 50 ~ 100 GPa. $BeBaH_8$ is a superconductor with T_S of 44 K at 100 GPa superior to BaH_{12} , and it remains dynamically stable at 15 GPa.



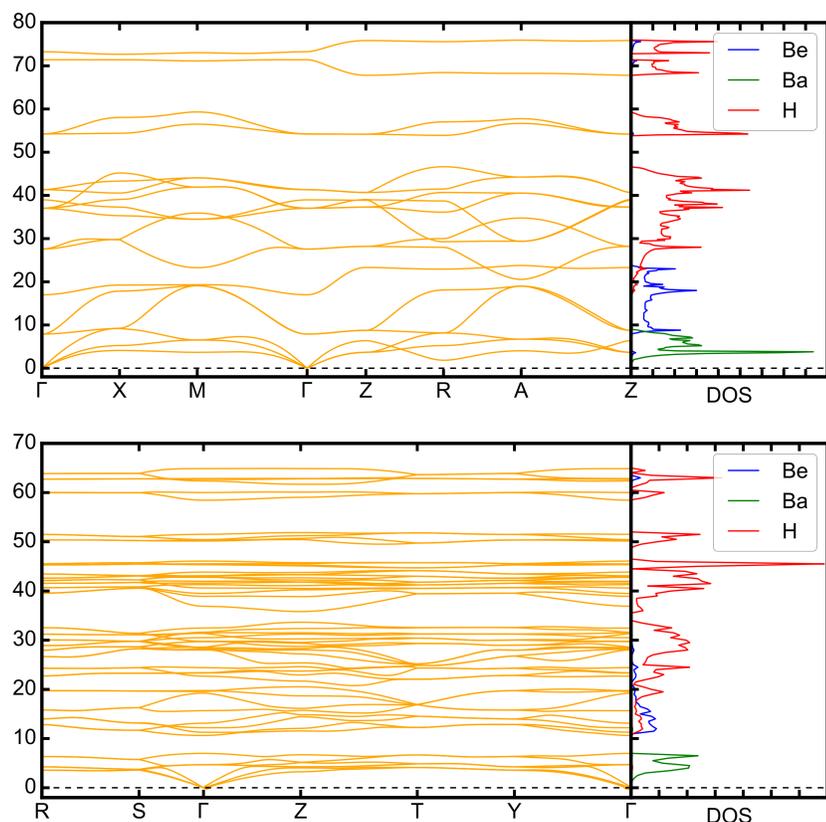
Crystal structure of BaH_{12} at 135 GPa including H_2 and H_3 molecules.

Phase diagram at 100 GPa

The pressure–composition phase diagram at 100 GPa is shown, along with the crystal structures of $BeBaH_4$ and $BeBaH_8$.



Lattice dynamics at 100 GPa



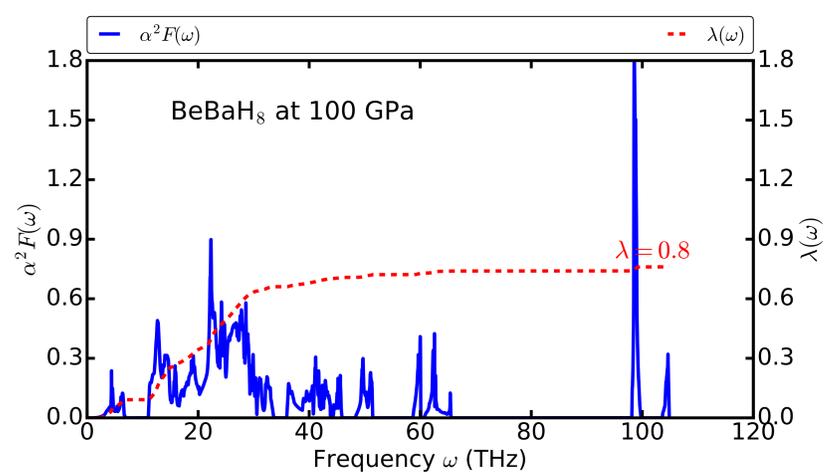
$BeBaH_4$ (upper panel) and $BeBaH_8$ (lower panel) are predicted to be dynamically stable at 100 GPa.

Supplementary information

The QR code goes to my twitter, where the poster is available and further discussions are welcome.

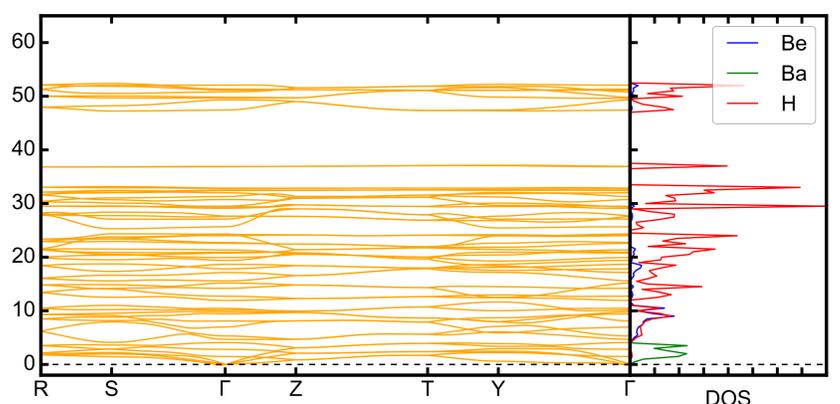


Superconductivity at 100 GPa



The electron-phonon coupling constant of $BeBaH_8$ is around 0.8 at 100 GPa. Using Eliashberg equation with Coulomb pseudopotential parameters (μ^*) of 0.1~0.13, the resulted T_S is 36-44 K at 100 GPa.

Survival at 15 GPa



$BeBaH_8$ is calculated to be dynamically stable down to 15 GPa in the harmonic approximation, indicating $BeBaH_8$ can be survived at very low pressures. However, its electron-phonon coupling constant at 15 GPa is reduced to 0.2.

Acknowledgments

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