The superconductivity in doped barium superhydrides

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Chen et al. [Nat Commun 12, 273 (2021)] synthesized barium superhydride BaH_{12} and reported its superconducting temperature T_S of 20 K at 140 GPa. BaH_{12} contains H2 and H3– molecular units, and show low density of states (DOS) at the Fermi level, which are responsible for the low T_S. Herein, light elements (A = Li, Be, etc.) are introduced into the barium superhydrides to reduce the molecular units and improve the DOS at the Fermi level. However, first-principles calculations find the crystal structure of BaH_{12} is dramatically changed upon doping, requesting investigations of the low-lying structures of A-Ba-H from scratch. We, therefore, use high-throughput crystal structure prediction to screen the low-lying structures under pressures up to 200 GPa. Combining the networking value that is correlated to T_S with the first-principles calculations, a list of superhydrides are predicted to be superconductors with T_S over BaH_{12}.

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