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Prediction of enhanced superconductivity in cyclo-H12Bi/Pb involving a resonant hydrogen structure

Hydrogen-based compounds demonstrate high-temperature superconductivity under pressure, offering promising avenues for exploring metal hydrides with elevated critical temperatures (c), while hydrides comprising H2 molecular units were previously deemed unfavorable.1 Searching for new forms of hydrogen within metal hydrides promised a route for developing novel high-temperature superconductors. In this study, we utilized the evolutionary algorithm alongside first-principles calculations to investigate the high-pressure crystal structure of the BinHn (=7–18) system. Notably, we discovered stable cyclo-H12Bi/Pb compounds in which the H12 resembles cyclohexanelike cyclo-H12 rings. These compounds are stable above 180 GPa and exhibit a higher c than BiH8 composed of H2 units. In cyclo-H12, the hydrogen has a slightly elongated intramolecular H-H length compared to BiH8, while the intermolecular H-H distance is much shorter than in H cages, forming a resonant structure. The resonance led to in-/out-of-plane vibration modes for the six H2 units in cyclo-H12, forming broad mid-frequency vibrational bands and boosting the electron-phonon coupling. These findings highlight the cycloform of hydrogen-based hydrides as promising candidates for high c superconductors, propelling further exploration of superconductivity in binary superhydrides with different forms of hydrogen.2

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