Highlights

Superconductivity - 2016

Superconductivity in metastable phases of phosphorus-hybride compounds under high pressure

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Reports on sulfur hydride attaining metallicity under pressure and exhibiting superconductivity at temperatures as high as 200 K have spurred an intense search for another room-temperature superconductor among hydrogen-rich compounds. Recently, compressed phosphorus hydride (phosphine) was reported to metallize at pressures above 45 GPa, reaching a superconducting transition temperature (Tc) of 100 K at 200 GPa.
However, neither the exact composition nor the crystal structure of the superconducting phase have been conclusively determined. This work reports an extensive study of the phase diagram of PHn (n=1-6) by means of *ab initio* crystal structure predictions using the minima hopping method (Fig. 1).
The results do not support the existence of thermodynamically stable PHn compounds, which exhibit a tendency for element decomposition at high pressure even when vibrational contributions to the free energies are taken into account.
Although the lowest energy phases of PH1,2,3 display Tc's comparable to experiments (Fig. 2), it remains uncertain if the measured values of Tc can be fully attributed to a phase-pure compound of PHn.

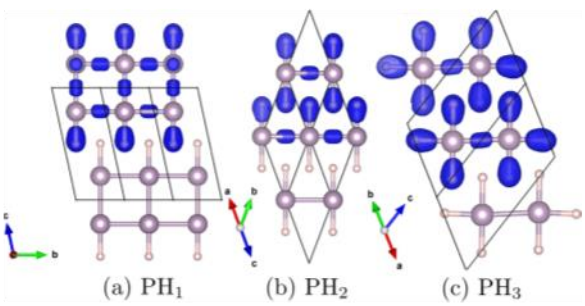

Fig. 1. Low-lying enthalpy structures found for different compositions under pressure 120 Gpa. The large and small spheres denote the P and H atoms, respectively.
The Electron Localization Function ad a fixed value of 0.8 is shown in the upper part of the figure.

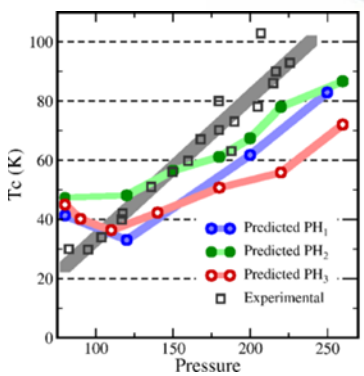

Fig. 2. Predicted Superconducting critical temperature for PH1, PH2 and PH3 as function of the pressure compared with experimental results.