Abstract Submitted
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Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure[1] JOSE FLORES LIVAS, University of Basel, MAXIMILIAN AMSLER, Northwestern University, ANTONIO SANNA, Max-Planck Institut fr Microstrukture Physics, CHRISTOPH HEIL, LILIA BOERI, Graz University of Technology, GIANNI PROFETA, Dipartimento di Fisica Universit degli Studi di LAquila , CRHIS WOLVERTON, Northwestern University, STEFAN GOEDECKER, University of Basel, E. K. U. GROSS, Max-Planck Institut fr Microstrukture Physics — Recently, compressed phosphine was reported to metallize at pressures above 45 GPa, reaching a superconducting transition temperature (T_c) of 100 K at 200 GPa. However, neither the exact composition nor the crystal structure of the superconducting phase have been conclusively determined. In this work the phase diagram of PH_n ($n = 1, 2, 3, 4, 5, 6$) was extensively explored by means of *ab initio* crystal structure prediction methods. The results do not support the existence of thermodynamically stable PH_n compounds, which exhibit a tendency for elemental decomposition at high pressure even when vibrational contributions to the free energies are taken into account. Although the lowest energy phases of $PH_{1,2,3}$ display T_c's comparable to experiments, it remains questionable if the measured values of T_c can be fully attributed to a phase-pure compound of PH_n.

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