Ab initio study of possible metastable occupation of tetrahedral sites in Palladium Hydride compounds

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Palladium hydrides are one of the rare examples of superconducting hydrides at ambient pressure. Even if their critical temperature is around 10 K, they are fascinating superconductors because of their inverse isotope effect: the palladium compound has a larger critical temperature than the hydrogen compound, in clear contradiction with standard electron-phonon superconductors. As shown by Errea et al.[1], this anomalous behavior is induced by the large anharmonicity of the hydrogen vibrations in the octahedral sites they occupy.

In recent times, in a controversial paper[2], high temperature superconductivity was observed in PdH compounds. The authors of the paper measure traces of superconductivity as high as at 54K for PdH if this compound is obtained through fast cooling in the synthesis. If the compound is obtained with slow cooling no superconductivity is observed. Their conclusion is that superconductivity depends strongly on the sites occupied by hydrogen atoms.

In this work we present first principles calculations including anharmonic effects within the stochastic self-consistent harmonic approximation (SSCHA)[3] in order to unveil the possible existence of dynamically stable structures with full or partial occupation of tetrahedral sites, which may be metastable. We discuss the implications of these possible structures in superconductivity.

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