

Abstract Submitted
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Elementary excitations and elusive superconductivity in palladium hydride – *ab initio* perspective. I. Paramagnons P. BUCZEK, MPI Halle, Germany, V. BORISOV, MLU Halle-Wittenberg, Germany, C. BERSIER, MPI Halle, Germany, S. OSPANIN, MLU Halle-Wittenberg, Germany, L. SANDRATSKII, MPI Halle, Germany, J.B. STAUNTON, University of Warwick, United Kingdom, E.K.U. GROSS, MPI Halle, Germany, I. MERTIG, MLU Halle-Wittenberg, Germany, A. ERNST, MPI Halle, Germany — Motivated by a experimental reports on possible high temperature superconductivity in palladium hydride [Tripodi *et al.*, *Physica C* **388-389**, 571 (2003)], we present a first principle study of spin fluctuations, electron-phonon coupling and critical temperature in PdH_x, 0 ≤ x ≤ 1. A prerequisite for any qualitative study of exchange-enhanced materials is the knowledge of spin flip fluctuation spectrum. It is generally believed [Berk & Schrieffer, *Phys. Rev. Lett.*, **17**, 433 (1966)] that the ferromagnetic-like paramagnons of Pd are destructive for the conventional, i.e. *s*-wave, superconductivity. We describe them using linear response time dependent density functional theory, recently implemented to study complex metals [Buczek *et al.*, *Phys. Rev. Lett.* **105**, 097205 (2010)] . We find that hydrogenation suppresses the intense spin fluctuations of pure Pd, driving it away from a magnetic critical point. Under the assumption of *s*-wave pairing, this could lead to the formation of the superconducting state. The *ab-initio* estimated electron-phonon coupling is strong enough to support superconductivity. Please look for the complementary contribution of Christophe Bersier.

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