

Abstract Submitted
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Elementary excitations and elusive superconductivity in palladium hydride – *ab initio* perspective. II. Phonons CHRISTOPHE BERSIER, PAWEL BUCZEK, MPI Halle, Germany, VLADISLAV BORISOV, SERGEY OSTANIN, MLU, Halle-Wittenberg, Germany, LEONID SANDRATSKII, MPI Halle, Germany, JULIE B. STAUTON, University of Warwick, United Kingdom, E.K.U. GROSS, MPI Halle, Germany, I. MERTIG, MLU, Halle-Wittenberg, Germany, ARTHUR 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 (T_c) in PdH_x , $0 < x < 1$. Our results described in terms of (i) electronic structure, (ii) phonon density of states and (iii) Eliashberg function show that the hydrogenation of Pd clearly enhance the electron-phonon coupling in this material. Assuming phonons to be the driving force for superconductivity, fcc Pd features a vanishingly small T_c , while for the stoichiometric $x = 1$ PdH the resulting T_c is around 10K in agreement with experiment. It is generally believed [Berk & Schrieffer, *Phys. Rev. Lett.*, **17**, 433 (1966)] that intense spin-&flip fluctuations of Pd are destructive for the conventional, i.e. *s*-wave, superconductivity. However, the H doping leads to a drastic reduction of spin-flip scattering. Please look for complementary presentation of Paweł Buczek.

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