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Improving the numerical description of high-pressure solid hydrogen phases

A variety of molecular solid hydrogen phases can be synthesized with diamond anvil cells between 100 and 400 GPa [1]. Raman and Infrared spectroscopy measurements have allowed the determination of the hydrogen phase diagram in this pressure range [2]. However, structural information on these phases is currently missing because of the low scattering efficiency of the hydrogen atom in X-ray diffraction experiments [3]. As such, numerical calculations are extremely valuable. Unfortunately, most Density Functional Theory (DFT) methods employed so far poorly describe the high-pressure molecular solid hydrogen phases [4]. Our objective has thus been to identify and use other methods presenting a better accuracy/computational cost ratio on these systems. We studied for this purpose the II-III phase transition occurring around 150 GPa experimentally. We found the Random Phase Approximation (RPA) to be in good agreement with reference calculations provided by quantum Monte Carlo methods [5,6]. We also found the hybrid DFT functional PBE0 containing 48% of Hartree-Fock exchange to be an accurate alternative. The relatively low computational cost of RPA and hybrid functionals, coupled with their enhanced accuracy, make them interesting tools for further improving the description of solid hydrogen phases by including effects currently missing in the numerical treatment, such as lattice vibrations and quantum nuclear effects.

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Affiliation de l'auteur principal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC)

Auteurs principaux: M. CONTANT, Damian (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC)); Dr HELLGREN, Maria (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC)); Dr CASULA, Michele (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC))

Orateur: M. CONTANT, Damian (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC))

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