Investigation of new metastable crystal structures of solid molecular hydrogen

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Under high enough pressures, hydrogen should form a crystal lattice. It is predicted that this hydrogen phase is a high-temperature superconductor. Three new metastable crystal structures have recently been predicted [1]. This information is sufficient to accurately calculate the superconducting transition temperature. Aiming that, we need to find the phonon spectra of these structures. In this work, we investigate the change in the structure and symmetry of hydrogen depending on pressure. We also obtain a cold isotherm for the newly predicted structures. The parameters of the calculation of the phonon spectrum of metastable solid molecular hydrogen are selected within the framework of the density functional perturbation theory method, which is implemented in the PHONon Quantum ESPRESSO software package. We use the Perdew–Burke–Ernzerhof exchange-correlation functional and a projector augmented wave pseudopotential from the Quantum ESPRESSO software package. We also select the parameters for calculating the dynamic matrix: the value of the basis of plane waves [2] and the grid of integration in the Brillouin zone. Current work shows that the new structure of hydrogen is quite stable due to symmetry, but the size of the unit cells can vary significantly. It also turns out that one cannot rely on the standard values of the listed parameters. On the basis of the results obtained, we discuss the applicability of the method used for calculating the transition temperature to the superconducting state.

[1] Saitov I M 2019 *JETP Lett.* **110** 206–210
[2] Kresse G and Furthmüller J 1996 *Phys. Rev. B* **54** 11169–11186