Anharmonic lattice dynamics calculations of crystalline hydrogen

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According to the theoretical predictions, crystalline hydrogen should have a number of unique properties [1]. In the present work, phonon calculations are performed for the phases of crystalline hydrogen that are stable at 100 K [2]. In addition to the conventional scheme based on the harmonic approximation, temperature and anharmonic effects are also considered. For calculation of harmonic force constants, finite displacement method is used. Forces are calculated in the VASP package [3–6]. Temperature and anharmonic effects are considered by using the model [7] as implemented in the DynaPhoPy package [8]. Ab-initio molecular dynamics simulations are performed in the VASP package. Corresponding force constants are used to calculate phonon spectra in the PhonoPy package [9]. Anharmonic and temperature effects lead to stabilization of the phases.

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