First-principles calculation of phonon properties of KDP crystal

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There are many defects formatted during the growth of potassium dihydrogen phosphate (KDP) crystal. This may have an important impact on the laser damage resistance of KDP crystals in ICF. We try to describe the crystal damage by studying the phonon properties. The lattice dynamics of KDP crystal with harmonic approximation and anharmonic effect are studied by using the first-principles DFT calculations. There are three large imaginary frequencies in the PE phase with harmonic approximation, which are the O-H stretching soft modes. The calculation of atomic participation ratio shows that B2 mode dominates the FE-PE phase transition. The three large imaginary frequency disappears with anharmonic effect, which indicates that the large displacement vibration of H atoms in PE phase. The calculation of displacement-displacement correlation function shows that the displacement of H atoms are one order of magnitude higher than other atoms. And H atoms participate in almost all vibration modes, only high-frequency vibrations are pure H vibrations in PE phase. The phonon calculation of the P-O stretching characteristic mode in 916 cm^{-1} of KDP crystal is consistent with the temperature-dependent Raman spectroscopy. The stretching vibration of H atoms may contribute significantly to the defects formatted and crystal damage of PE phase KDP.