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Ab initio investigation of phonon spectra in GdLiF4 compound under hydrostatic pressure

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Abstract

Employing density functional theory (DFT) within the generalized gradient approximation, the GdLiF4 structure has been studied for a pressure range from 0 to 12 GPa. The influence of pressure on the lattice vibrational spectrum of the scheelite phase (I41/a, Z = 4) has been evaluated by means the "direct" approach, i.e., using force constants calculated from atomic displacements. As a result the Raman and infrared modes have been identified and their dependencies on pressure have been investigated and compared with available experimental data. It has been found that instability of the crystal structure appears at pressures above 6 GPa. © 2014 Pleiades Publishing, Ltd.

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