

擬調和振動子近似による振動自由エネルギーの第一原理計算

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First Principles Calculations of Vibrational Free Energy Estimated by the Quasi-Harmonic Approximation

The quasi-harmonic approximation is a powerful tool for predicting the vibrational free energy using the first principles calculations. This method with the phonon density of state shows reliable estimation of the thermal expansion and the relative stabilities of SiC polytypes. For the binary systems, we derived a cancelling condition of the vibrational free energy change due to the phase separations within the first order approximation in terms of the nearest bond pair interaction.

Keywords: Einstein lattice, phonon, thermal expansion, SiC polytypes, binary