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Phonon structures and IR intensities in strained BaTiO₃ ALDO RAELIARIJAONA, University of Arkansas, HUXIANG FU — While soft modes and structural instability in cubic ferroelectrics have been well studied, the vibration properties in structurally stable phases are relatively less understood, however. Here we have carried out first-principle calculations, using density-functional perturbation theory, to determine the phonon structures and IR intensities at gamma point for tetragonal Barium titanate under different in-plane strains, in which lattice parameter ranges from 3.93 Å to 3.80 Å. We find that some modes shift strongly with the inplane strain, while other modes show surprisingly little change. The response of IR intensity is also revealed to be mode-dependent. The microscopic insight for these behaviors is examined.

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