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First-Principles Investigation of Vibrational Properties of $CaTiO_3$ Crystal SUBENIA MEDEIROS, MAEVA ARAUJO, UFERSA — The structural, electronic, vibrational, and optical properties of perovskite $CaTiO_3$ in the cubic, orthorhombic, and tetragonal phase are calculated in the framework of density functional theory (DFT) with different exchange-correlation potentials by CASTEP package. The calculated band structure shows an indirect band gap of 1.88 eV at the Γ-**R** points in the Brillouin zone to the cubic structure, a direct band gap of 2.41 eV at the $\Gamma - \Gamma$ points to the orthorhombic structure, and an indirect band gap of 2.31 eV at the $\mathbf{M} - \Gamma$ points to the tetragonal phase. I have concluded that the bonding between Ca and TiO_2 is mainly ionic and that the TiO_2 entities bond covalently. Unlike some perovskites the $CaTiO_3$ does not exhibit a ferroelectric phase transition down to 4.2 K. It is still known that the $CaTiO_3$ has a static dielectric constant that extrapolates to a value greater than 300 at zero temperature, and the dielectric response is dominated by low frequency ($\nu \approx 90\text{cm}^{-1}$) polar optical modes in which cation motion opposes oxygen motion. Our calculated lattice parameters, elastic constants, optical properties, and vibrational frequencies are found to be in good agreement with the available theoretical and experimental values. The results for the effective mass in the electron and hole carriers are also presented in this work.

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