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Comparative Study Between GGA and LDA Approximation Using First- Principles Calculations of Structural, Electronic, Optical and Vibrational Properties of CaTiO₃ Crystal SUBENIA MEDEIROS, MAEVA ARAUJO, Universidade Federal Rural do Semi-Árido — The structural, electronic, vibrational, and optical properties of perovskite CaTiO₃ 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 Γ - Γ points to the orthorhombic structure, and an indirect band gap of 2.31 eV at the **M** - Γ points to the tetragonal phase. It is still known that the CaTiO₃ 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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