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First-Principles Calculations of Structural, Electronic and Optical Properties of $CaTiO_3$ Crystal SUBÊNIA MEDEIROS, JUSCIANE SILVA, Universidade Federal Rural do Semi-Árido - UFERSA, EUDENILSON ALBUQUERQUE, Universidade Federal do Rio Grande do Norte - UFRN, VALDER FREIRE, Universidade Federal do Ceará - UFC — 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 Γ−Γ points to the orthorhombic structure, and an indirect band gap of 2.31 eV at the MΓ 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. 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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