Ab initho Study of electronic and thermodynamic properties of CaTiO3

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Structural and electronic properties of CaTiO3 in cubic phase calculated. The calculations have been done in the framework of density functional theory and with local density approximation (LDA) and generalized gradient approximation (GGA). After optimizing structural properties of CaTiO3 and checking ability of our method in calculating structural and electronic properties, thermodynamics properties of CatiO3 have been calculated using Gibbs package. The study of thermodynamic properties of materials is of great importance in order to extend our knowledge about their specific behaviors when put under severe conditions such as high pressure and high temperature environment. In order to precede the thermodynamic calculations, one needs an accurate knowledge of equation of state and related thermodynamic properties. After the convergence tests, the calculated total energies were fitted to the murnaghan equation of state. Our calculated lattice parameters and bulk modulus indicating a good agreement with experimental results. The thermal properties were determined in the temperature range 0 to 1000 k, quasi-harmonic model remains fully valid. The pressure effect is studied in the 0 to 60 Gpa range. The calculated variations of specific heat in different temperature and pressure showed the Debye T3 behavior at low temperatures and saturating at high temperatures which are consistent with experimental results.

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