

Abstract

The theoretical study in detail to explain the external pressure effects from (0.0 to 25) GPa with the difference of 2.5GPa on electronic-structure ,structural-stability, band-gap-engineering & with the use of CASTEP code check the effect of pressure on optical-properties of LN, depend upon ab-initio density-functional-theory (DFT), with ultra soft pseudo-potential & exchange-correlation-functional GGA-PBE, is accessible. it is noticed from structural band that the valence- band (VB) top normally controlled through orbital electrons of Nb-4d & O-2p & by increasing the pressure the band-gap is reducing between (3.542 - 2.905) eV. Reduction in electronic band-gap by increasing the external pressure help us to explain the Decreasing trend of the electronic band-gap with increase of external pressure is explained with the help of total-density of states (TDOS) & elemental-partial-density of states (EPDOS). Further the pressure is increased more than 25GPa then the structure stability reduces significantly. We have also investigated reduction of band-gap effect on the optical properties of LN. The optical results which are calculated refractive-index (RI), absorption-function (AF) & the reflectivity-rate (RR) are expand with the increase in pressure. With the increase in pressure the red shift & blue shift (major-Plasmon-peaks) shown by absorption-spectra & it is very important prove of reduction of band-gap. So, the both electronic-structures & optical-properties of LN can be changed by applying the pressure.