ABSTRACT

First principles calculation, based upon Density Functional Theory (DFT), with Generalized Gradient Approximation (GGA) and ultra-soft pseudo potential (USP) are made to investigate structural, electronic, and optical properties of lead titanate ($PbTiO_3$) after nitrogen doping. Lattice parameters and band gap of pure lead titanate are found in good agreement with literature, and for doped lead titanate, reduction in band gap is reported. Nitrogen doping changes phase structure of pure $PbTiO_3$ from cubic to pseudo-cubic tetragonal. Likewise, addition of nitrogen in oxygen sites creates new states at Gemma symmetry points shifting band gap from indirect to direct. For detailed overview of density of states of $PbTiO_3$, graphs of partial density of states (PDOS) and elemental partial density of states (EPDOS) are plotted and exhibit the coupling of O-2*p*-states with Ti-*d*-states, however, lead (Pb) has minimum contribution in density of states. In addition, optical properties- such as real and imaginary part of dielectric function, refractive index, reflection, absorption, energy loss function, and extinction coefficient- of pure and doped lead titanate have also been computed. Shifting of absorption edge towards lower energy states means there is red shift in doped PTO which makes nitrogen doped lead titanate an attractive nominee for its use in optoelectronic domains.