Abstract

In this work, we adopted density functional theory to analyze the changes in opto-electronic properties of wide band gap of pure and N_2 doped $BaZrO_3$ perovskite. The Generalized gradient approximations were employed to evaluate the structural, electronic and optical properties. Different concentrations of N_2 doping at O_2 lattice sites showed the increasing trend of density of states in the conduction band which slightly moved towards the Fermi level. Hence a systematic decreasing trend of band gap was observed with doping. The optical properties confirmed that the doped compound would be appropriate for absorbing electromagnetic radiations in the visible and IR region of electromagnetic spectrum.