ABSTRACT

The structural, electronic and optical response of strontium titanate with doping of lithium (Li), potassium (K) and beryllium (Be) have been investigated. Our computational analysis is carried out with code-key of CASTEP through DFT (density functional theory), to put forward summations under exchange-correlation functional PBE-GGA (Perdew-Burke-Ernzerhof-Generalized Gradient Approximations) and USP (ultra soft pseudo potential). We have analyzed different characteristics of pure and doped compounds i.e. the electronic band structure (BS), partial density of states (PDOS), total density of states (TDOS) and their outcome on DF (dielectric function). The partial replacement of Sr-atoms with the Li-, K- and Be-atoms restyle lattice constant to a certain extent and remodeled the band gap of intrinsic STO with the occurrence of newly formed *k*-points. There is an increase in bandgap of pure STO with Li and K doping from 1.792eV to 1.897eV and to 1.888eV, respectively. But in case of Be doping its value decreases to 1.620eV. This change in bandgap is explained by the partial and total density of states. For pure and doped STO, the bandgap nature remains unchanged i.e. indirect bandgap. This doping has also influenced the optical properties and absorption edge shifts towards lower energy from 0.32eV to 0.02eV (red shift) for Be-doped STO. We have also observed an increase in static refractive index (2.49 to 4.6). A positive change is observed in the doping of Li, K and Be in STO through electronic and optical characteristics and proves this much powerful agent for optoelectronic devices.