ABSTRACT

$SrZrO_3$(SZO) doped with calcium and barium is subjected to density functional theory with GGA-PBE to elaborate the basic, electronic and optical properties of these perovskites. TDOS and PDOS is applied to investigate the effect on electronic structure and ultimately on optical properties of SZO perovskites. A limited substitution of strontium with Ca or Ba in SZO results in variation of structural framework which leads to the advancement of new sites at the points of symmetry by PDOS and ultimately followed the band gap reduction is seen. It has also been observed that the indirect band gap changes to direct band gap after the addition of Ca or Ba in the SZO. Optical properties of true and impure SZO are completely correlated with the electronic calculation. A significant change in band gap and ultimately in optical properties in SZO after doping with Ba and Ca clears both type of materials as a strong candidate for its use in optoelectronic devices.