ABSTRACT

A comprehensive theoretical study, based on density functional theory (DFT) with GGA-PBE, of structural, electronic and optical properties of beryllium (Be), magnesium (Mg) and lithium (Li) doped $SrZrO_3$ is presented. The doping has a great impact on the electronic structure and subsequently optical properties have been analyzed and enlightened with TDOS and PDOS. Structural parameters change by slight replacement of strontium (Sr) atom with Be, Mg and Li in $SrZrO_3$, separately. Reduction in electronic band gap is perceived after the doping of Be and Mg but after the doping of Li an increased band gap is detected. We have also noticed that the indirect band gap of pure $SrZrO_3$ is altered to the direct band gap after doping of Be and Mg but the nature of band gap remains direct for Li doped system. The optical properties of the pure and doped $SrZrO_3$ are consistent with their electronic determinations. The performance of revised electronic and optical properties of SZO after doping of alkali (Li) and alkaline (Be and Mg) metals would be suitable in optoelectronic devices.