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First-Principles Investigation of Structural, Electronic, and Optical Response of $SnZrO_3$ with Al Inclusion for Optoelectronic Applications

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In this study, the first-principles calculation which is grounded on the density functional theory is employed to conclude the structural, optical, and electronic properties of pure and Al-incorporated $SnZrO_3$ (SZO). The effect of Al on structural, optical, and electronic properties using generalized gradient approximation and ultra-soft pseudo potential is discussed. The aim of this study is to explore the change in structural, optical, and electronic properties due to minimal insertion of impurity into pristine system. Al is doped at Sn site which is more favorable as compared to Zr site because of the stability condition of cubic perovskites. The captivation of Al at Sn site in SZO embellished the electronic band gap energy E_g by creating new gamma points. E_g is reduced from 1.778 to 1.250 eV after the inclusion of minimal quantity of Al impurity. Not only the band gap is reduced due to Al inclusion but also the nature of E_g is altered from direct to indirect. The total density of states and partial density of state are explained this behavior as the *p*-state is responsible for drastic reduction of band gap. The change in electronic properties also affects the optical properties such as complex dielectric function, absorption, reflection, and refractive index. The study reveals that the index of refraction increases from 3.43 to 3.82 and an increase in dielectric function is also observed. Thus, Al-doped SZO is a curious material for optoelectronic device.

Keywords: band gap, density functional theory, density of states, absorption, refractive index.