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Pressure Dependence of Structural, Electronic, and Optical Properties of $Be_{0.25}Zn_{0.75}O$ Alloy

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The structural, electronic, and optical properties of $Be_{0.25}Zn_{0.75}O$ alloy as a function of the pressure have been investigated by using the first-principles density functional theory within the generalized gradient approximation. The results show that the lattice constants decrease and the band gap increases with increasing pressure. The valence band maximum moves to lower energy, whereas the conduction band minimum moves to higher energy with increasing pressure, so the band gap broadens. The dielectric constant $\varepsilon_1(0)$ and zero frequency refractive index $n(0)$ decreases monotonically with increasing pressure. The variation of imaginary part of the dielectric function, extinction coefficient, absorption coefficient, and electron energy loss function with different pressure are well described. The curve shape for optical parameters is almost unchanged with increasing pressure, but all the peaks moves to higher energy. Our results provide a theoretical reference for $Be_{0.25}Zn_{0.75}O$ alloy at different pressures to achieve better ZnBeO performance in optoelectronic devices.

Keywords: DFT, $Be_{0.25}Zn_{0.75}O$ alloy, high pressure, electronic properties, optic properties, refractive index.