Influence of K-doping on the optical properties of ZnO by first principle studies

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Optical properties of K-doped ZnO were studied using the density functional method within the local spin-density approximation LSDA. In this work, we present the influence of the potassium (K) on optical properties using the wurtzite structure and a supercell of 32 atoms, by calculating the dielectric function to understand the optical interband transitions in diverse configurations with the substitution of Zn by one and two transition metal (TM) atoms into ZnO. We show that the band gap of K-doped ZnO decrease with the rise in doping level, the intensity of K-doped ZnO is blue emission. The latter is going to be analyzed in details.