n-type to p-type conductivity insights in Ag and Sb doped ZnO for electronic and optoelectronic applications

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Abstract: Recent investigations of p-type semiconductor materials have been gained most research interest due to their extraordinary physical and chemical properties as well as worthy applications in advanced electronic and optoelectronics. To this end, the electronic and optical properties of undoped, Ag and Sb doped ZnO are performed in the framework of density functional theory (DFT) implemented with generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE). Interestingly, it is clearly observed that n-type ZnO has been transformed to p-type ZnO simultaneously doping of Ag and Sb on the Zn site in ZnO. The acceptor doping levels are generated above the valence band which implicitly indicates the p-type nature of Ag and Sb-doped ZnO. The band gap narrowing exhibited at lower doping concentrations, however, the band gap widening is happen at higher doping attributed due to Burstein Moss effect. Further analysis of optical and electronic properties confirmed enhanced of optical and electrical conductivity due to introduced of additional charge carrier by dopants. Thus, the findings of this study will be helpful for design and fabrication of high efficient electronic and optoelectronic devices as well as experimental exploration of Ag and Ag-Sb doped ZnO.

Keywords: p-type ZnO, acceptor doping, DFT, photoconductivity, optoelectronic.

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