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Comparative first-principles analysis of electronic and absorption calculations of mono- and co-doped ZnO with trivalent ions Gd+3 and Al+3

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Abstract

In this paper, the energitics, electronic and absorption properties analysis of ZnO doped and co-doped with trivalent ions Gd+3 and Al+3 have been performed using first-principles calculations with the hybrid functional theory. The results show that the energetic stability can be easily prepared the desirables Gd-, Al-doped and Gd/Al-codoped ZnO at O-rich conditions. In addition, the incorporation of Gd+3 and Al+3 into ZnO lattice creates shallow donor states around Fermi level in the conduction band minimum from mainly Al-3s and Gd-6s states, which offers good electronic properites with significant improvements for the Gd-doping compared to other dopants and pure ZnO. The results show that the absorption peaks of Al-doped and Gd/Al-codoped ZnO have a blue-shift compared with pure ZnO. However, the absorption of Gd/Al-codoped ZnO is slighly higher than that of pure and monodoped ZnO in the visible and infrared zone. Finally, these results confirm that trivalent ions doped-ZnO has n-type conductivity.

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