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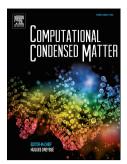
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Effect of nitrogen doping on electronic and optical properties of ZnO sheet: DFT+U study

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Abstract

Structural, optical and electronic properties of bulk and two-dimensional (2D) nanostructure of pure and N-doped ZnO have been investigated using density functional theory and the Hubbard U (DFT + U_d + U_p) method. Here, we considered four models of graphene like pure and N-doped ZnO (one layer and two layers) and compared them to bulk ZnO. This study evaluates the influence of Hubbard U parameter on p-orbital electrons of nitrogen ($U_{p,N}$). Our optical and electronic analyses of $U_{p,N}$ = 7eV show nitrogen is a deep acceptor for bulk N-doped ZnO, which is in good agreement with some theoretical and experimental reports. Results show the existence of N atoms cannot lead to hole conductivity in ZnO bulk and graphene like layers of N-doped ZnO.

Keywords: DFT, Hubbard U, N-doped ZnO, graphene like, dielectric function

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