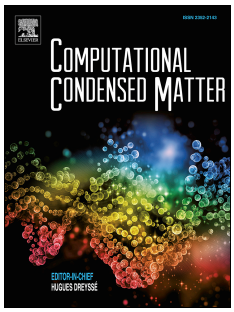
Accepted Manuscript



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

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PII: S2352-2143(18)30033-9

DOI: 10.1016/j.cocom.2018.03.001

Reference: COCOM 140

To appear in: *Computational Condensed Matter*

Received Date: 11 February 2018

Revised Date: 3 March 2018

Accepted Date: 4 March 2018

Please cite this article as: S.S. Parhizgar, J. Behestian, Effect of nitrogen doping on electronic and optical properties of ZnO sheet: DFT+U study, *Computational Condensed Matter* (2018), doi: 10.1016/j.cocom.2018.03.001.

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

PACS: 71.15.Mb, 71.20.-b, 71.55.-I, 78.c20.-e