First principles LDA+U study of structural, electronic, elastic and optical properties of Mn doped wurtzite ZnO

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The structural, electronic, elastic and optical properties of pure and Mn-doped ZnO with a wurtzite structure were calculated by using first-principles calculation based on density functional theory (DFT) with local density approximation (LDA) [1] plus Hubbard U (DFT–LDA+U) method [2]. This latter represents the theoretical framework to deal with strongly correlated materials to predicted successfully the electronic properties of such materials. The wurtzite ZnO system is then doped with Mn at different sites. The obtained results were discussed and compared with earlier works.
Keywords ; Wurtzite ZnO; LDA+U; Density functional theory (DFT).

1. *Clark S. J., Segall M. D., Pickard C. J., Hasnip P. J., Probert M. J., Refson K., Payne M. C.* First principles methods using CASTEP// Zeitschrift fuer Kristallographie. -2005.-**220**.-P. 567-570.
2. *Yaakob M. K., Hussin N. H., Taib M. F. M., Kudin T. I. T.,Hassan O. H., Ali A. M. M.,1, Yahya M. Z. A.* First Principles LDA+U Calculations for ZnO Materials // Integrated Ferroelectrics. -2014. **-155**.-P. 15–22.