Theoretical Study about the effect of Mn concentration on the electronic structure of $Ga_{(1-x)}Mn_{(x)}N$ diluted magnetic semiconductor.

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The aim this work is to contribute to the understanding of the effect of structural disorder on the electronic structure of $Ga_{(1-x)}Mn_xN$ diluted magnetic semiconductor (DMS). We have constructed several hexagonal wurtzite supercell models of 32 and 96 atoms [1] to simulate this system with different Mn contents (x=0.02; 0.06; 0.08 and 0.18), and compared our first principles calculations with the experimental available data [2]. Our supercell periodic calculations were performed with the CRYSTAL06 program package[3]. Becke's three-parameter hybrid nonlocal exchange functional combined with the Lee-Yang-Parr gradient-corrected correlation functional (B3LYP) was used. Our results show a reasonable agreement with the experimental energy band gap, the gap falls with the increase of Mn concentration, due to formation of intermediary energy levels within the band gap near the valence band and can be related to an increase of the electronic disorder of the material. On the other hand, we find for a ~8% Mn concentration that the clusterization of Mn atoms is energetically favored in comparison with a dilutes picture. Nevertheless for higher Mn contents the system seems to prefer a more dilute Mn distribution.

Keywords: $Ga_{1-x}Mn_xN$, Diluted magnetic semiconductor, DFT.

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[1] A. Gulans, R. A. Evarestov,.I. Tale, C. C. Yang, Phys.Stat.So.l **7**, 2525. **(**2005).
[2] J. H. D. da Silva, D. M. G. Leite, A.Tabata, A. A. Cavalheiro, J. Appl. Phys. **102**, 063526. **(**2007)
[3] R. Dovesi, V. R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N. M. Harrison, I. J. Bush, Ph. D'Arco, M. Llunell, Crystal 2006 User's Manual_University of Turin, Turin, (2006).

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