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# Electronic structure of Mn-doped GaN

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**Abstract** – A theoretical method to simulate the structural and electronic properties of hexagonal wurtzite $Ga_{1-x}Mn_xN$ with different Mn contents (x = 0.00, 0.02, 0.05, 0.07, 0.08 and 0.18) is proposed. The periodic quantum-mechanical method is based on density functional theory at B3LYP level using CRYSTAL03 computer code. The structural models were obtained from Rietveld refinement of the undoped and Mn doped GaN X-ray diffraction data.

The GaN is a promising and coveted material for studies due to its semiconductor property and its characteristic region of light emission between visible blue and ultraviolet [1]. The physical properties of the Mn doped GaN still present several unexplained aspects, however the material has a great potential in technological applications, mainly in spintronics [2].

In this work, a computational study of the electronic structure of the diluted magnetic semiconductor (DMS) $Ga_{1-x}Mn_xN$, with x = 0.00, 0.02, 0.05, 0.07, 0.08 and 0.18, was performed in order to improve the understanding of its structural and electronic properties. In the calculations, the influence of Mn is indirectly calculated using the experimental lattice parameter variation in the $Ga_{1-x}Mn_xN$ with different Mn contents.

The measured structure parameters of $Ga_{1-x}Mn_xN$ thin films prepared by reactive rf magnetron sputtering [3] were used in the calculations. The resulting electronic structures were compared with experimental data of the absorption edge of the material. This study was based on simulations carried out with the CRYSTAL03 program [4], based in the Density Functional Theory with hybrid functional B3LYP.

**Table 1:** Lattice Parameter ***a***, ***c*** (Å), ***u***, ***c/a***, volume (Å$^3$), experimental and calculated band gap (eV).

| $Ga_{1-x}Mn_xN$ | ***A*** | ***c*** | ***u*** | ***c/a*** | ***V*** | $gap_{exp}$ | $gap_{DFT}$* |
|---|---|---|---|---|---|---|---|
| x = 0.00 | 3.2039 | 5.2041 | 0.398 | 1.624 | 46.263 | 3.23 | 3.60 |
| x = 0.02 | 3.2070 | 5.2042 | 0.395 | 1.623 | 46.343 | 3.17 | 3.60 |
| x = 0.05 | 3.2111 | 5.2137 | 0.395 | 1.624 | 46.557 | 3.10 | 3.57 |
| x = 0.07 | 3.2161 | 5.2242 | 0.397 | 1.624 | 46.796 | 2.91 | 3.49 |
| x = 0.08 | 3.2219 | 5.2220 | 0.404 | 1.621 | 46.945 | 2.88 | 3.42 |
| x = 0.18 | 3.2316 | 5.2489 | 0.446 | 1.624 | 47.472 | 2.07 | 3.32 |

*this work.

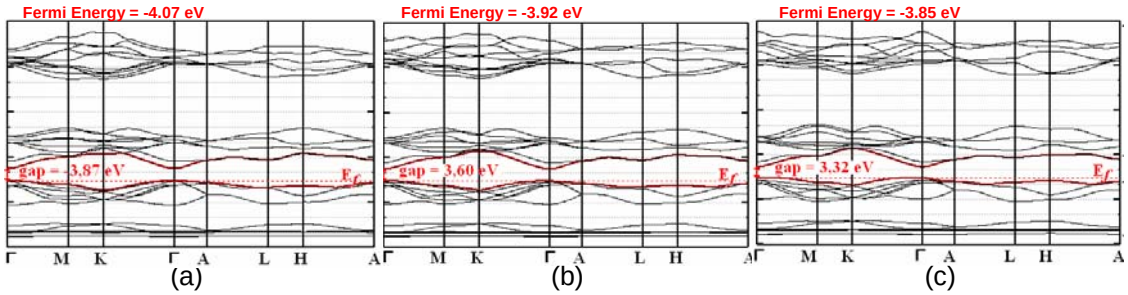


**Figure 1:** Band Estructure for the (a) $\mathbf{GaN_{Teor.}}$; (b) $Ga_{1-x}Mn_xN$ com x = 0 e (c) $Ga_{1-x}Mn_xN$ com x = 0.18.

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## References

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