First principles studies of magnetic properties of wurtzite $Ga_{0.9375}TM_{0.0625}N$, (TM=V, Cr, Mn, Fe, Co, Ni)

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9.7 cm

The aim of this work is study of the influence of V,Cr,Mn,Fe,Co and Ni on the electronic and magnetic properties of $Ga_{1-x}TM_xN$ in wurtzite structure. The electronic structure of zinc-blende phase were studied recently [1, 2]. In this work we present the results obtained by ab initio method based on the density functional theory within generalized gradient approximation (GGA) and the pseudopotential method [3]. The calculations were performed for 32-atoms supercell model. The transition metal was substitute in the place of Ga. For Cr, Fe, Ni and Mn the electronic states at the Fermi level are 100% spin polarized, however for V and Co atoms the densities of states at the Fermi level are partially polarized.

References

[1] E. Kulatov et al., Phys. Rev. B **66**, 045203 (2002)
[2] S.-C. Lee et al., J. Magn. Magn. Mater. **310**, e732 (2007)
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13.4 cm

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