First principles studies of magnetic properties of wurtzite \( \text{Ga}_{0.9375}\text{TM}_{0.0625}\text{N}, \) (TM=V, Cr, Mn, Fe, Co, Ni)

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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 \( \text{Ga}_{1-x}\text{TM}_x\text{N} \) 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


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