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Magnetic and electronic properties of V doped GaN: An *ab initio* study

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Abstract – First-principles spin-polarized calculations have been performed in order to investigate the effect of varying V concentration in $Ga_xV_{1-x}N$ (x=0.0625, 0.125, 0.25 and 0.5) on the electronic and magnetic properties of V doped GaN in the wurtzite structure. The calculations of the structural properties and the density of states (DOS), within the framework of the Density Functional Theory (DFT) as it is implemented in the wien2k program, were carried out. The results obtained were in agreement with previous studies: V-3d orbitals form an impurity band separated from the valence states of the host GaN for dilute V concentration.

The possibility to manipulate the spin of the electron, as well as the charge, opens up fascinating routes for processing information and data storage. This is particularly exciting in terms of semiconductor spintronics, where conventional charge-based electronics could be replaced with devices possessing both spin and charge functionality. Dilute magnetic semiconductors (DMS)—semiconductors doped with a few per cent of magnetic atoms— are being actively investigated in the development of spintronic devices. While there has been much work on the III–V DMS materials, notably (In,Mn)As and (Ga,Mn)As, their ferromagnetic Curie temperatures (*Tc*) (90K for (In,Mn)As [1] and 172K for (Ga,Mn)As [2]) are too low for practical applications. The realization of practical commercial or mobile devices will require the development of semiconductors that can retain their ferromagnetic magnetic properties above room temperature. As a result, significant research effort has been focused on developing alternative DMS materials with higher Curie temperatures [3].

First-principles spin-polarized calculations have been performed in order to investigate the effect of varying V concentration in $Ga_xV_{1-x}N$ (x=0.0625, 0.125, 0.25 and 0.5) on the electronic and magnetic properties of V doped GaN in the wurtzite structure. A supercell approach was employed. We chose a fraction of the GaN semiconductor crystal and replacing one of the Ga-atoms by a V-atom impurity in the supercell structure. Only this replacement was made and no other disorder was introduced in the material. The calculations of the structural properties and the density of states (DOS), within the framework of the Density Functional Theory (DFT) as it is implemented in the wien2k program [4], were carried out. We have used the hybrid energy functional B3PW91 for the correlated electrons. This functional have predicted very accurate structural properties as the bulk modulus [5]. A parallel discussion is made between those and the results obtained using the Generalized Gradient Approximation (GGA) of Perdew-Burke-Ernzerhof (PBE 96) [6] for the exchange and correlation potential. The results obtained were in agreement with previous studies: V-3d orbitals form an impurity band separated from the valence states of the host GaN for dilute V concentration. It is likely that the V atoms are ferromagnetic ordered forming a magnetic semiconductor although the V is a nonmagnetic material in the natural phase. V-doped GaN is shown to possess a total magnetic moment of 2.0 μ_B per supercell. The results indicate that the ferromagnetic ground state is originated from the strong hybridization between V-3d orbitals and N-2p orbitals. This work shows that the V-doped GaN is a promise magnetic semiconductor (MS). This study gives new clues to the fabrication of MS. We presented a detailed discussion about these results.

References

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