An ab-initio investigations on the magnetic properties of (Co, N) doped ZnO and (Co, C) doped GaN

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Gallium Nitride and Zinc Oxide are the most actively investigated semiconductors for applications in optoelectronics. The physical and chemical properties of these materials are highly suitable for high temperature environment and for space applications. Dietl et al [1] have predicted that transitional metal doping in these semiconductors would make them suitable for ferromagnetism at room temperature. After that several investigations have been carried out in analyzing the properties of TM doped ZnO & GaN as Dilute Magnetic semiconductors (DMS) for the spin based applications. We have investigated the magnetic properties of cobalt doped ZnO and GaN with an additional anion element. Our experimental results showed room temperature magnetism in both (Co, N) doped ZnO and (Co, C) doped GaN systems.

In the study of (Co,N) doped ZnO, a super cell of 72 atoms have been generated to perform lower percentage of doping (3%) and the spin based electronic structures were obtained by performing the self-consistent calculation using the FP-LAPW method as implemented in WIEN2K code. The calculations were carried out for different combinations of Co occupying the Zn site and N occupying O site like - i) Co and N bonded together and ii) Co and N are far from each other. These combinations reveal that the spin polarized Co atom increases the magnetic moment of the shortest bonded atom with not much change in the total magnetic moment of the system ($4\mu_B$). The energetically favorable position is when Co and N are bonded together; there is a mutual exchange of spin between Co – N in their p-d hybridization which results in slight increase in the magnetic moment at Co site (2.67 μ_B). In this configuration, the magnetic moment of the N and O in the tetrahedral bonding with Co is found to be 0.36 μ_B and 0.12 μ_B respectively. The effect of O and Zn vacancies in the magnetic properties of the (Co, N) doped ZnO system hae also been investigated. Interestingly, the creation of Zn vacancy has found to increase the magnetic moment of the bonded anions. The calculations revealed that with creation of defects and additional (N) doping one can control the magnetic moments in ZnCoO system.

In the case of (Co, C) doped GaN, the electronic structures were obtained by performing self-consistent calculation using TB-LMTO method. Like the previous case, the calculations were carried out for different positional substitutions and defect formations. The introduction of carbon in the GaCoN system is found to increase the magnetic moment of cobalt (2.95 μ_B). Either the distance between Co and C or the site occupancy is found to have significant role in determining the magnetic moment of the system. Even if there is an underestimation of the bandgap in the used scheme (LDA), the positional occupancy of the Co and C tends to change the electrical behavior i.e magnetic with half-metallic or semiconducting nature in this system. The Co – C –Co bonding is found to be energetically favorable to yield magnetism in the (Co, C) doped GaN system.

Reference:

1. T. Dietl, H. Ohno, F. Matsukura, J. Cibert and D. Ferrand, Science 287(2000) 1019.