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Electronic structures and valence band splittings of transition metals doped GaNs

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Abstract

For a practical viewpoint, presence of spin splitting of valence band in host semiconductors by the doping of transition metal (TM) ions is an essential property when designing a diluted magnetic semiconductors (DMS) material. The first principle calculations were performed on the electronic and magnetic structure of 3d transition metal doped GaN. V, Cr, and Mn doped GaNs could not be candidates for DMS materials since most of their magnetic moments is concentrated on the TM ions and the splittings of valence band were negligible. In the cases of Fe, Co, Ni, and Cu doped GaNs, on the contrary, long-ranged spin splitting of valence band was found, which could be candidates for DMS materials.

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Keywords: Diluted magnetic semiconductor; GaN; Transition metals; Valence band splitting; First principle calculations

1. Introduction

In diluted magnetic semiconductors (DMSs), according to Dietl et al.'s [1] explanation, doped transition metal (TM) ions produce the localized magnetic moments and give rise to the spin splitting of valence band of host semiconductors. The long range exchange interaction between the TM ions and the delocalized hole stabilizes the ferromagnetic alignment of TM ions and the spin splitting of the valence band. The latter is finally used for spin injection in spintronic devices.

Theoretical studies that aimed to design a new DMS material have focused mainly on the ferromagnetic interaction between TM ions [2–5]. The high temperature ferromagnetism, however, is a necessary condition not a sufficient one: a TM doped semiconductor can be used for a DMS material only when the materials have spin polarized carriers above room temperature although the material exhibits high temperature ferromagnetism.

This study has focused mainly on the valence band splitting of host semiconductor due to the doping of TM ions using first principle calculations. GaN was chosen as a host material and 3d TMs from V to Cu were used as dopants.

2. Computational detail

All the calculations was performed using the plane-wave basis code, the Vienna *ab initio* simulation package (VASP) [6,7], based on density-functional theory and using ultra-soft pseudopotentials [8]. The generalized gradient approximation (GGA) parametrized by Perdew and Wang [9] was used for the exchange-correlation potential. To enhance the magnetic moment and magnetic energies, the interpolation formula proposed by Vosko et al. [10] was used. Ga 3d state was treated as a semi-core state. The energy cutoff was up to 800 eV and a $8 \times 8 \times 8$ Monkhorst–Pack special k-points mesh was used for the integration of Brillouin-zone. The geometry was optimized by quantum mechanical force.

The zinc blende structure of GaN was used and assumed that the same results also hold for the wurtzite structure. The calculated lattice parameter of the zinc blende GaN was 4.53 Å, which agrees well the experimental value [11].

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The periodic supercell approach having 64 atoms was used. Transition metal elements were assumed to occupy Ga site, which corresponds to 3.125 at% of concentration. TMs used were V, Cr, Mn, Fe, Co, Ni, and Cu.

3. Results and discussion

First principle calculations showed that the ferromagnetic phases were stable for all systems as shown in Fig. 1. Square dots and circles represent the total and the TM projected magnetic moments, respectively. The highest magnetic moment of 5 μ_B was obtained for Fe doped GaN. Total magnetic moment of Mn doped GaN was 4 μ_B that are consistent with other ab-initio calculations [12,13]. While change of total magnetic moment follows Hund's rule, TM projected magnetic moments behave differently. The differences in total and projected moments for V, Cr, and Mn were smaller, 0.445 μ_B in average, the differences in Fe, Co, Ni, and Cu larger, 1.318 μ_B. In the viewpoint of the formation of delocalized spin carriers, V, Cr, and Mn doped GaN cannot be used since most of their spins are concentrated at the TM ions.

The induced magnetic moments of N atoms are shown in Fig. 2 as a function of distance from the TM ions. For comparison the induced moments of As in GaAs:Mn, which has been known to be the only one successful DMS, were plotted as well. The systems whose magnetic moments were concentrated at TM ions, no induced moment was observed except for the first neighboring N atom. The origin of ferromagnetism in these systems is predicted to be short-ranged such as double exchange, which cannot be used for DMS material. On the contrary, the systems exhibiting less-concentrated magnetic moments resulted in the long-ranged splitting of valence band in host semiconductors. When comparing with GaAs:Mn, the extent of induced magnetic moments of late transition metals in GaN host are comparable or large than that of GaAs:Mn, which means that the stronger p–d hybridizations occurred.

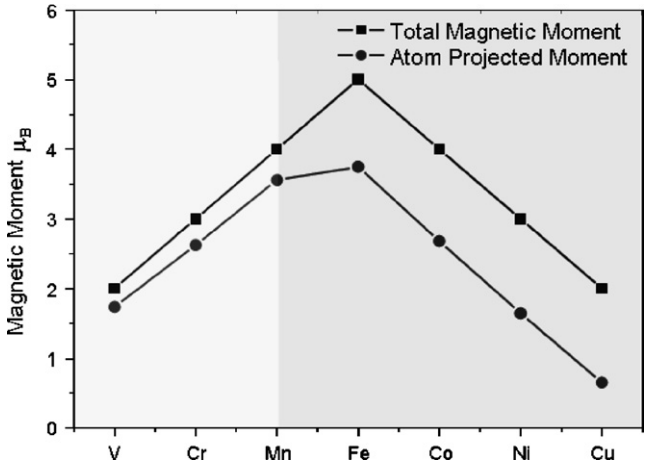

Fig. 1. Calculated total (square) and TM projected (circle) magnetic moment of 3.125% TM doped GaN.

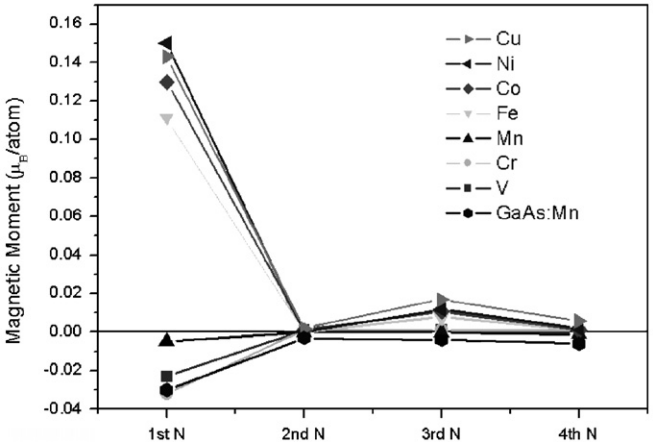

Fig. 2. Induced magnetic moments of nitrogen. 1st, 2nd, 3rd, and 4th represent the distances from the magnetic ion.

4. Conclusion

The first principle calculations were performed on electronic and magnetic properties of transition metal doped GaN. Early transition metals such as V, Cr, and Mn showed that the most of its magnetic moments were concentrated at TM sites. The effect of valence band splitting was very small. Late transition metals from Fe to Cu, on the contrary, substantial fraction of magnetic moments were distributed up to 4th neighboring N atoms. The long ranged interaction was predicted in the case of late TM ions. These systems can be candidates for DMS materials if the systems exhibit room temperature ferromagnetism. There has been a report that ferromagnetic phases are not stable phases in the cases of Fe, Co, Ni, and Cu-doped GaNs [14]. More works are needed to predict the feasibility of the calculation results.

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