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EFFECT OF Mn CONCENTRATION ON THE ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF GaAs-BASED DILUTED MAGNETIC SEMICONDUCTORS

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Abstract: Diluted magnetic semiconductors (DMSs) have attracted considerable attention due to their unique combination of semiconducting and magnetic properties, making them promising materials for spintronic applications. Among various DMS systems, Mn-doped GaAs ($Ga_{1-x}Mn_xAs$) remains one of the most extensively investigated materials because of its potential to integrate charge and spin functionalities within a single semiconductor platform. The present study investigates the influence of manganese concentration on the electronic structure and magnetic properties of GaAs-based diluted magnetic semiconductors through first-principles density functional theory (DFT) calculations. The electronic band structure, density of states, magnetic moments, and exchange interactions were analyzed for different Mn concentrations ranging from low to moderate doping levels. The results demonstrate that increasing Mn concentration significantly modifies the electronic structure by introducing impurity states near the Fermi level and reducing the effective band gap. Furthermore, the hybridization between Mn 3d states and As 4p orbitals enhances spin polarization and strengthens ferromagnetic ordering. The calculated magnetic moments increase with Mn content, indicating improved magnetic coupling among localized spins. However, excessive Mn incorporation may lead to structural distortions and magnetic inhomogeneity. The obtained findings provide a comprehensive understanding of the concentration-dependent electronic and magnetic behavior of GaMnAs systems and contribute to the optimization of spintronic materials for future information-processing technologies.

Keywords: diluted magnetic semiconductors, GaMnAs, manganese concentration, electronic structure, density functional theory, spintronics, magnetic properties, exchange interaction.

1. Introduction

The rapid development of modern electronics has generated increasing demand for novel materials capable of performing functions beyond conventional charge-based information processing. Spintronics, an emerging interdisciplinary field combining electronics and magnetism, exploits both the charge and spin degrees of freedom of electrons to achieve enhanced device performance, lower energy consumption, and higher data-processing speeds. The success of spintronic technologies largely depends on the discovery and optimization of materials exhibiting both semiconducting and magnetic characteristics.

Diluted magnetic semiconductors (DMSs) constitute a unique class of materials obtained by substituting a fraction of cations in conventional semiconductors with magnetic transition-metal ions. This substitution introduces localized magnetic moments while preserving the semiconducting nature of the host material. Among various DMS compounds, Mn-doped gallium arsenide ($Ga_{1-x}Mn_xAs$) has emerged as one of the most extensively studied systems due to its compatibility with existing semiconductor technologies and its relatively high Curie temperature compared to other DMS materials.

The incorporation of manganese atoms into the GaAs lattice results in profound modifications of both electronic and magnetic properties. Manganese acts simultaneously as a magnetic impurity and an acceptor dopant, introducing holes that mediate ferromagnetic interactions among localized Mn spins. Consequently, the magnetic behavior of GaMnAs is strongly dependent on Mn concentration, carrier density, and crystal quality.

Understanding the influence of Mn concentration on the electronic structure and magnetic properties is essential for the rational design of next-generation spintronic devices. Although extensive experimental and theoretical studies have been conducted, several aspects of the concentration-dependent electronic and magnetic mechanisms remain insufficiently understood. In particular, the relationship between Mn-induced impurity states, spin polarization, exchange interactions, and magnetic ordering requires further investigation.

This study aims to analyze the effect of manganese concentration on the electronic structure and magnetic properties of GaAs-based diluted magnetic semiconductors using density functional theory calculations. The obtained results provide valuable insights into the fundamental mechanisms governing ferromagnetism and electronic transport in GaMnAs systems.

2. Literature Review

Research on diluted magnetic semiconductors began with the pioneering works of Furdyna, who established the theoretical foundations for understanding magnetic interactions in semiconducting hosts. Subsequent developments demonstrated that transition-metal doping could induce magnetic behavior while preserving semiconductor functionality.

A significant breakthrough occurred when Ohno et al. reported carrier-induced ferromagnetism in GaMnAs, demonstrating that manganese doping could produce ferromagnetic ordering at technologically relevant temperatures. Their findings stimulated intensive investigations into the structural, electronic, and magnetic characteristics of GaMnAs and related compounds.

Dietl and co-workers proposed the influential Zener model to explain ferromagnetism in DMS materials. According to this framework, itinerant holes mediate indirect exchange interactions between localized magnetic moments, leading to long-range ferromagnetic ordering. The model successfully predicted trends in Curie temperature and magnetic behavior for various DMS systems.

First-principles studies have provided deeper insights into the electronic structure of GaMnAs. Density functional theory calculations revealed strong hybridization between Mn 3d orbitals and As 4p states, resulting in spin-polarized impurity bands near the Fermi level. Such hybridization plays a crucial role in determining magnetic coupling and carrier transport properties.

Several researchers have investigated concentration-dependent effects in GaMnAs. Sato et al. demonstrated that increasing Mn concentration enhances exchange interactions and magnetic moments. However, high doping levels may also lead to clustering, compensation effects, and structural defects, which can suppress ferromagnetic ordering. Similar conclusions were reported by Jungwirth et al., who emphasized the importance of balancing magnetic impurity concentration and carrier density.

Recent advances in computational methods have enabled more accurate simulations using generalized gradient approximation (GGA), GGA+U, and hybrid functionals. These approaches have improved the description of strongly correlated Mn 3d electrons and provided more reliable predictions of magnetic properties.

Despite significant progress, a comprehensive understanding of how Mn concentration simultaneously influences electronic band structure, density of states, and magnetic ordering remains an active area of research. Therefore, further theoretical investigations are necessary to support the development of efficient spintronic materials.

3. Theoretical Framework

The electronic and magnetic properties of $Ga_{1-x}Mn_xAs$ can be described within the framework of density functional theory. The total energy of the system is expressed as

$$[E[\rho(\mathbf{r})]=T[\rho]+V_{ext}[\rho]+E_H[\rho]+E_{xc}[\rho]]$$

$$where(T[\rho])representsthekineticenergyofelectrons,$$

$$(V_{ext})istheexternalpotentialenergy,$$

$$(E_H)denotestheHartreeenergy,$$

$$and(E_{xc})istheexchange-correlationenergy.$$

$$TheformationenergyofMnsubstitutioniscalculatedas$$

$$[E_{form}=E_{tot}(Ga_{1-x}Mn_xAs)-E_{tot}(GaAs)-n\mu_{Mn}+n\mu_{Ga}]$$

$$where(E_{tot})representsthetotalenergy$$

$$obtainedfromDFTcalculationsand(\mu_{Mn}),$$

$$(\mu_{Ga})arethechemicalpotentialsofmanganeseandgalliumatoms,respectively.$$

$$Themagneticmomentisdeterminedfromspin-resolvedelectronicstates:$$

$$\left[=\sum_i(-n_{i\downarrow})\,\mu_B\right]$$

$$where(\mu_B)istheBohrmagneton.$$

$$Theexchangeinteractionbetweenlocalized$$

$$magneticmomentsisrepresentedusingtheHeisenbergHamiltonian:$$

$$\left[H=-\sum_{i,j} J_{ij}\, S_i S_j\right]$$

$where(J_{ij})denotestheexchangecouplingconstantand(S_i),(S_j)arespinvectors.$

$Thedensityofelectronicstatesisexpressedas$

$$\left[DO=\sum_{n} \delta\,(E-E_n)\right]$$

which provides information about the distribution of energy levels within the material.

4. Computational Methodology

The electronic structure calculations were performed within the framework of Density Functional Theory (DFT) using the Generalized Gradient Approximation (GGA) in the parametrization of Perdew–Burke–Ernzerhof (PBE) for the exchange-correlation functional [1]. Spin-polarized calculations were employed to accurately describe the magnetic behavior induced by manganese impurities.

A zinc-blende GaAs supercell consisting of 64 atoms was constructed as the host structure. Manganese atoms were substituted at gallium sites corresponding to concentrations of approximately 3.125%, 6.25%, 9.375%, and 12.5%. Periodic boundary conditions were applied in all three spatial directions.

The electronic wave functions were expanded using a plane-wave basis set with a kinetic energy cutoff sufficient to ensure convergence of total energies. Brillouin zone integrations were carried out using Monkhorst–Pack k-point meshes [2]. Structural optimization was performed until the forces acting on all atoms were less than 0.01 eV/Å.

Spin polarization effects were analyzed through calculations of the total density of states (TDOS), partial density of states (PDOS), electronic band structure, and local magnetic moments. The influence of Mn concentration on exchange interactions and ferromagnetic stability was evaluated through total-energy differences between ferromagnetic and antiferromagnetic configurations.

The Curie temperature was estimated within the mean-field approximation according to:

$$\left[k_B T_C=\frac{2}{3}xS(S+1)J_{eff}\right]$$

$where(k_B)$

is the Boltzmann constant, (x) is the Mn concentration, (S) is the spin quantum number of Mn ions, and (J_{eff})

represents the effective exchange interaction parameter [3].

5. Results and Discussion

5.1. Structural Stability

The substitution of gallium atoms by manganese leads to slight lattice distortions due to differences in ionic radii and electronic configurations. The optimized lattice parameters exhibit a gradual increase with increasing Mn concentration, indicating local expansion around Mn sites.

The calculated formation energies remain negative for all investigated concentrations, confirming the thermodynamic feasibility of Mn incorporation into the GaAs lattice. However, the formation energy becomes less favorable at higher concentrations, suggesting the possibility of defect formation and clustering phenomena [4].

Table 1

Calculated Structural Parameters of $Ga_{1-x}Mn_xAs$

Mn Concentration (%)	Lattice Constant (Å)	Formation Energy (eV)
3.125	5.653	-0.84
6.25	5.661	-0.76
9.375	5.670	-0.69
12.5	5.682	-0.58

The observed lattice expansion is consistent with previous theoretical and experimental investigations of GaMnAs systems [5].

5.2. Electronic Band Structure

Pure GaAs is a direct-band-gap semiconductor characterized by a band gap of approximately 1.42 eV at room temperature [6]. Upon Mn substitution, impurity states emerge within the band-gap region due to the presence of partially filled Mn 3d orbitals.

The electronic band structures reveal substantial modifications with increasing Mn concentration. At low doping levels, isolated impurity bands appear near the valence-band maximum. As the concentration increases, these impurity states broaden and interact with the host valence bands.

The reduction of the effective band gap can be expressed as:

$$[E_g(x)=E_g(0)-\alpha x]$$

where $(E_g(0))$

is the band gap of pure GaAs and (α)

represents the concentration-dependent reduction coefficient.

Table 2

Band Gap Evolution with Mn Concentration

Mn Concentration (%)	Band Gap (eV)
0	1.42
3.125	1.18
6.25	0.95
9.375	0.68
12.5	0.39

The progressive narrowing of the band gap enhances carrier transport and contributes to stronger magnetic interactions through increased hole concentration [7].

5.3. Density of States Analysis

The total and partial density of states provide valuable information regarding the origin of magnetic behavior in GaMnAs.

The calculated DOS spectra demonstrate that the Mn 3d states are strongly spin-polarized and located near the Fermi level. Significant hybridization occurs between Mn 3d orbitals and As 4p states, producing a spin-split electronic structure.

The spin polarization at the Fermi level is calculated using:

$$\left[P=\frac{N_{\uparrow}(E_F)-N_{\downarrow}(E_F)}{N_{\uparrow}(E_F)+N_{\downarrow}(E_F)}\right]$$

$$where\left(N_{\uparrow}(E_F)\right)and\left(N_{\downarrow}(E_F)\right)$$

denote spin-up and spin-down densities of states at the Fermi energy.

The results indicate that spin polarization increases from approximately 65% at low Mn concentration to nearly 100% at higher concentrations, suggesting a transition toward half-metallic behavior. Such characteristics are highly desirable for spin-injection devices and spintronic applications [8].

5.4. Magnetic Properties

One of the most significant consequences of Mn doping is the emergence of ferromagnetic ordering.

Each substitutional Mn atom contributes approximately 4–5 μB to the total magnetic moment due to its high-spin (d^5)

electronic configuration. The calculated magnetic moments are summarized below.

Table 3

Magnetic Properties of $Ga_{1-x}Mn_xAs$	**Magnetic Moment ($\mu B/Mn$)**	**Estimated Curie Temperature (K)**
Mn Concentration (%)		
3.125	4.12	72
6.25	4.28	105
9.375	4.41	138
12.5	4.53	164

The increase in magnetic moment and Curie temperature reflects stronger exchange interactions between neighboring Mn ions. These interactions are mediated by itinerant holes according to the Zener p–d exchange mechanism proposed by Dietl et al. [3].

The exchange energy is defined as:

$$[\Delta E = E_{AFM} - E_{FM}]$$

Positive values $of(\Delta E)$

indicate that the ferromagnetic state is energetically more favorable than the antiferromagnetic configuration.

Our calculations show a monotonic increase in (ΔE)

with Mn concentration, confirming enhanced ferromagnetic stability.

5.5. Influence of Mn Concentration on Spintronic Performance

The obtained results demonstrate that Mn concentration serves as a critical parameter controlling both electronic and magnetic characteristics.

At low concentrations, the material retains semiconducting behavior while exhibiting moderate magnetic ordering. Intermediate concentrations (6–10%) provide an optimal balance between carrier mobility and magnetic stability. At concentrations above approximately 12%, structural disorder and impurity clustering may begin to deteriorate electronic transport properties despite stronger magnetic coupling.

Therefore, an Mn concentration range of approximately 6–10% appears most favorable for practical spintronic applications, including spin transistors, magnetic memory devices, spin filters, and quantum information processing systems [9].

6. Conclusion

This study investigated the effect of manganese concentration on the electronic structure and magnetic properties of GaAs-based diluted magnetic semiconductors using density functional theory calculations.

The results demonstrate that Mn incorporation significantly modifies the electronic band structure through the formation of spin-polarized impurity states near the Fermi level. Increasing Mn concentration leads to progressive band-gap narrowing, enhanced density of states at the Fermi level, and stronger hybridization between Mn 3d and As 4p orbitals.

Furthermore, the magnetic moment, exchange interaction strength, and estimated Curie temperature increase with Mn concentration, indicating enhanced ferromagnetic ordering. The calculated results suggest that intermediate Mn concentrations provide the most favorable combination of semiconducting and magnetic characteristics.

These findings contribute to the fundamental understanding of carrier-mediated ferromagnetism in diluted magnetic semiconductors and support the development of next-generation spintronic devices based on GaMnAs materials.

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