

## Short Communication

### Review on Available Theoretical Models for Room Temperature Ferromagnetism in Dilute Magnetic Semiconductors

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Dilute magnetic semiconductors have been attracting scientific community due to their wide array of applications like spintronics devices such as nano-magnetic memories, nano-sensors, etc. The researchers have gathered a large amount of experimental data over the past few decades with varied perceptions into the origin of ferromagnetism in dilute magnetic semiconductors. Some investigators found the room temperature ferromagnetism (RTFM) because of metallic groups; whereas others revealed the same because of the substitution of doped transition metals (TM) into the host milieu and called it as semi-magnetic semiconductors. Some of them also found paramagnetic behaviors at room temperature, however, achieved RTFM after annealing in vacuum/H<sub>2</sub>/air or any other medium. Theoretical models like Ruderman-Kittel-Kasuya-Yosida (RKKY), Zener, bound magnetic polaron (BMP) were also developed to investigate the same, but to some extent, confusion remains about which interaction mechanism is responsible for the observed intrinsic type of RTFM. The theoretical modeling is among utmost imperative analysis in the research progression. It helped to understand the conceptual and quantifiable knowledge of the origin of ferromagnetism in the dilute magnetic semiconductors. Furthermore, it may offer the essential path to cultivate an efficacious approach for the manufacturer of these materials. The present paper epitomizes various theoretical models viz RKKY model, Zener model, mean-field Zener model and BMP model that elucidate the RTFM in dilute magnetic semiconductors. The study reveals, among various BMP models, magnetic ordering is most reliant in the finding the RTFM, and quite successful to explicate ferromagnetic exchange coupling amid the TM local moments in dilute magnetic semiconductors.

**Keywords:** Room temperature ferromagnetism (RTFM), Ruderman-Kittel-Kasuya-Yosida (RKKY) model, Zener model, Mean-field Zener model and bound magnetic polaron (BMP) model.

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## 1. INTRODUCTION

The diluted magnetic semiconductors (DMS) are considered as functional materials in spintronic devices, circumscribe typical semiconductors that exhibit a considerable portion of atoms surrogated by transition metals (TM). These TM produce localized magnetic moments in the semiconductor matrix which are frequently originated from their respective *3d* or *4f* un-wrap shells. An energetic spin-dependent articulation among the localized states and bands causes humongous splitting of the spin electronic states, spin-disorder scattering and evolution of magnetic polarons that can be controlled, probed and escorted towards collective spin glass ordering accordingly [1]. Moreover, researches have been extended to DMS based on wide gap oxide semiconductor systems, such as TiO<sub>2</sub>, SnO<sub>2</sub>, In<sub>2</sub>O<sub>3</sub>, etc. These oxide-based DSM (O-DMSs) have captivated much acclaim due to prospects in spintronics and magneto-optoelectronic applications [2, 3].

Various theoretical and experimental research findings have been reported in literature on the ferromagnetic, paramagnetic, antiferromagnetic and spin glass properties of TM-doped DMS [4, 5]. Sikam et al. [6] investigated pristine ZnO and Zn<sub>1-x</sub>Fe<sub>x</sub>O in both empirical and theoretical characteristics. They used

combustion method to prepare Zn<sub>1-x</sub>Fe<sub>x</sub>O ( $x = 0.000, 0.0625, \text{ and } 0.125$ ) nanoparticles. The structural properties, electronic band structure, density of states and magnetic property of pristine ZnO and Zn<sub>1-x</sub>Fe<sub>x</sub>O were also theoretically explored by means of density functional theory with Local Density Approximation (LDA), General Gradient Approximation (GGA), with Hubbard model scheme (U). Meng et al. [7] suggested that the Co-doped In<sub>2</sub>O<sub>3</sub> is favorable for RTFM; as they implemented first-principle spin-polarized density functional theory calculations to prove the magnetic interactions of Co atoms in In<sub>2</sub>O<sub>3</sub>. An et al. [8] investigated both experimentally and theoretically the structural, magnetic and transport properties of the films. They summarized that the variation of Ms with Fe doping has a strong relationship with the localization radius  $\xi$  of carriers and the characteristic hopping temperature  $T_0$ , signifying that the change of localization impact can extraordinarily influence the FM order of the (In<sub>1-x</sub>Fe<sub>x</sub>)<sub>2</sub>O<sub>3</sub> films.

Amidst these theoretical and experimental findings still the origin of RTFM is subjected to more clear insight. It becomes indispensable to compare experimental results with the expected observations for the various theoretical models for RTFM in these DMS materials.

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In view of this, the present paper illuminates a short review on a few models which set forth to expound the ferromagnetism in magnetic semiconductors.

## 2. THEORETICAL MODELS FOR FERROMAGNETISM IN DMS

### 2.1 The RKKY Model

The RKKY (Ruderman-Kittel-Kasuya-Yosida) model [9] elucidates the magnetic interaction amid solitary localized magnetic and delocalized conduction band electrons. Due to RKKY interaction, conduction electrons near the magnetic ion get magnetized and act as an effective field to impact the polarization of neighboring magnetic particles, with the oscillatory polarization rotting with distance from the magnetic ions and causing indirect super exchange interaction (RKKY) between two magnetic ions on closest or next closest magnetic neighbors. This coupling brings about a parallel (ferromagnetic) or an anti-parallel (antiferromagnetic) setting of moments dependent on separation of the interacting atoms. This RKKY interaction is proficient when a high concentration of delocalized carriers exists in the host material.

This model cannot be realized easily for the magnetic semiconductors which archetypally contain dilute subsystem of localized magnetic spins and an even more dilute gas of free carriers [10].

### 2.2 Zener Model

Zener postulates the model of FM driven by the exchange interaction amongst carriers and localized spins. When transition atoms dissolved in a metal or alloy that generally contains only completed inner shells then the transition atoms have ordered positions with no nearest neighbors of each other. In such alloys, there would be no direct exchange of electrons amongst d shells. Hence, the FM coupling by means of conduction electron should offer ascent to FM at low temperatures [11].

In the Zener model, the direct interaction between d shells of the contiguous TM atoms (super-exchange) prompts an antiferromagnetic configuration of the d shell spins in light of the fact that the TM-d shell is half-filled. Then again, the indirect coupling of spins via the conduction electrons has a tendency to adjust the spins of the incomplete d shells in a FM way. It is only when these rules over the direct super-exchange coupling amongst neighboring d shells are observed. The drawback of the model is that it gives an approximate estimation of ferromagnetism driven by the exchange interaction among free carriers and localized magnetic moments, perceived at critical ferromagnetic temperatures in DMS materials. The Zener model disregards essential impacts identified with the character of the ferromagnetic order in these systems, probably mediated by the wandering nature of the free carrier spins.

### 2.3 The Mean Field Zener Model

Dietl et al. [12] proposed the mean-field Zener model which is based on the original model of Zener and the RKKY interaction. When contrasted with the

RKKY collaboration, the mean-field Zener model considers the anisotropy of the carrier-mediated exchange interaction allied with the spin-orbit coupling in the host material and furthermore the carrier correlation. In the process, it propounds the imperative impact of the spin-orbit coupling in the valence band in finding the magnitude of  $T_c$  and direction of the simple axis in  $p$ -type ferromagnetic semiconductors. It shows a hole mediated FM interaction between localized spins in magnetic semiconductor. With a specific end goal to induce the long ranged FM, the holes should have been spatially delocalized or feebly localized [12, 13].

### 2.4 Bound Magnetic Polaron Theory

The bound magnetic polaron (BMP) model is an imperative methodology for elucidating the ferromagnetic ordering in the TM doped oxide semiconductors. BMP is an assemblage of electrons (or holes) bound to impurity atoms via exchange interactions within an orbit [14]. Reliant to the system, these interactions render carriers parallel or anti-parallel to the magnetic impurity. The parallel and anti-parallel alignments contrast in energies, leading to non-zero spin flip energy states, which is an idiosyncrasy of BMPs. As  $s$ - $d$  exchange energy exceeds  $k_B T$ , the mutual alignment of ions and carriers results in a ferromagnetic “bubble” i.e. “collective” regime which occurs normally at low temperatures whereas at elevated temperatures the spins of magnetic ions are not continual and lead to non-zero magnetization via spin fluctuations i.e. “fluctuation” regime within respective carrier orbit.

The BMP magnetic ordering temperature is reliant on the nature of interactions among charge carriers and atomic spins. Durst et al. [15] computed exchange parameters based on the polaron-pair model that accounts the interaction amongst BMP pairs through mutual interstitial zone. Such zones are essential for carrier mediated ordering of every BMP [16].

In the formation of BMPs, if  $s$ - $d$  interactions are feeble and donor bands are comparatively high, then collective phase is perceived merely at low temperatures whereas if additional localized valence bands intricate, then  $p$ - $d$  interaction becomes robust to endure mutual phases even at upper temperature ranges.

Based on exchange interaction amid the atomic spin moment of dopant ions and extremely interrelated constricted impurity bands for  $n$ -type DMS, Coey et al. [16] suggested a model. They demonstrated schematically the interactions within oxides, in which the defects such as oxygen vacancies act as a source of electrons. When the concentration of electrons that are aligned with characteristic Bohr radii upsurges their individual orbits, they spread out into constricted impurity bands. If there are adequate magnetic spins, the electrons are absolutely spin polarized and resulting ferromagnetic ordering due to indirect exchange interaction intermediated by carriers [17, 18].

## 3. CONCLUSIONS

The models conferred here illustrate that the pertinent characteristics of TM doped DMS and their heterostructures can be inferred qualitatively. The RKKY

interactions generally prevail over the direct exchange coupling among adjacent local magnetic moments as well as magnetic dipole-dipole coupling. Zener model suggests that the magnetic interaction is diffused from one spin to another through indirect exchange interaction which is intermediated by a conduction electron of doped TM ion. The mean field Zener approximation is applicable for long-range character of the ferromagnet-

ic interactions in terms of combined effects of spin-orbit interaction and confinement.

The BMP model evinces that RTFM in TM doped DMS materials is mainly caused by the development of BMP localized acceptor sites that polarize the TM atoms by the exchange field with the localized holes. In this way these interactions restraint the magnitude and character of magnetic and transport anisotropies.

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## Огляд доступних теоретичних моделей для феромагнетизму за кімнатної температури в розбавлених магнітних напівпровідниках

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Розбавлені магнітні напівпровідники привертають увагу наукового співтовариства завдяки широкому спектру застосувань, таким як пристрої для спітроніки, наномагнітні пристрої пам'яті, наносенсори і т.д. Дослідники збрали велику кількість експериментальних даних за останні кілька десятиліть з різними уявленнями про походження феромагнетизму у розбавлених магнітних напівпровідниках. Деякі дослідники виявили феромагнетизм за кімнатної температури (RTFM) через металеві групи; в той час як інші виявили його через заміну легованих перехідних металів у середовищі матриці і назвали їх напівмагнітними напівпровідниками. Деякі з них також виявили парамагнітну поведінку при кімнатній температурі, однак досягали RTFM після відпалу у вакуумі/Н<sub>2</sub>/повітрі або будь-якому іншому середовищі. Теоретичні моделі, такі як моделі Рудермана-Кіттеля-Касуя-Йосіда, Зенера та зв'язаного магнітного поляруну (BMP), також були розроблені для дослідження феромагнетизму, але певною мірою залишається незрозумілим, за який механізм взаємодії відповідає спостережуваний внутрішній тип RTFM. Теоретичне моделювання є одним з першочергових імперативних аналізів у дослідженні. Це допомагає зрозуміти походження феромагнетизму у розбавлених магнітних напівпровідниках. Крім того, моделювання може запропонувати визначальний шлях для вироблення ефективного підходу до виготовлення цих матеріалів. У даній роботі розглянуто різні теоретичні моделі, а саме модель РККУ, модель Зенера, середньопольова модель Зенера і модель BMP, що пояснюють RTFM в розбавлених магнітних напівпровідниках. Дослідження показує, що серед різних моделей магнітне впорядкування є найбільш залежним у знаходженні RTFM, тому досить успішно можна пояснити феромагнітні обмінні зв'язки на тлі локальних моментів перехідних металів в розбавлених магнітних напівпровідниках.

**Ключові слова:** Феромагнетизм за кімнатної температури (RTFM), Модель Рудермана-Кіттель-Касуя-Йосіда (РККУ), Модель Зенера, Середньопольова модель Зенера, Модель магнітного поляруну (BMP).