

Semiconductor Magnets: The Origin of Ferromagnetism

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A dilute magnetic semiconductor (DMS) is a semiconductor material that has been made ferromagnetic through doping with transition metal cations at low concentrations.^{1,2} In some of these materials, ferromagnetism is intimately interwoven with the electrical properties of the material, leading to phenomena such as electrical control of magnetism and magnetic tuning of conductivity.^{3,4,1} These properties have generated much interest in these material for applications such as high density non-volatile memory and spintronic computation.⁵

All currently known DMSs have Curie temperatures that are well below room temperature (e.g. **Table I**). As a result, any device that depends on their ferromagnetic properties will work only at low temperatures. A thorough understanding of the physical mechanism by which ferromagnetism arises in these materials could lead to the discovery of DMSs with higher Curie temperatures.

Material	Curie Temperature (K)
$\text{Ga}_{0.94}\text{Mn}_{0.06}\text{P}$	60
$\text{Ga}_{0.89}\text{Mn}_{0.11}\text{As}$	180
$\text{In}_{0.90}\text{Mn}_{0.10}\text{As}$	90

Table I: Curie temperatures of some DMS materials⁶

Because the solubility of Mn in GaAs and InAs is less than 1%, all of these DMSs are metastable and they must be made by non-equilibrium techniques such as molecular beam epitaxy.²

In these materials, Mn formally enters as Mn^{3+} cations replacing Ga^{3+} or In^{3+} ions, but it is thought that the Mn^{3+} centers convert to Mn^{2+} ions by accepting an electron from the filled valence band, thus creating a hole in this band. Ferromagnetism arises in Mn-doped GaAs through an indirect mechanism, in which parallel alignment of electron spins on separate Mn^{2+} ions (\mathbf{S}_1 and \mathbf{S}_2 in **Figure 1**) is mediated by the spin-carrying itinerant holes.⁷

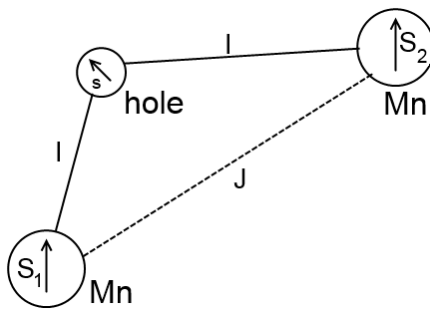


Figure 1. Carrier-mediated ferromagnetic coupling.

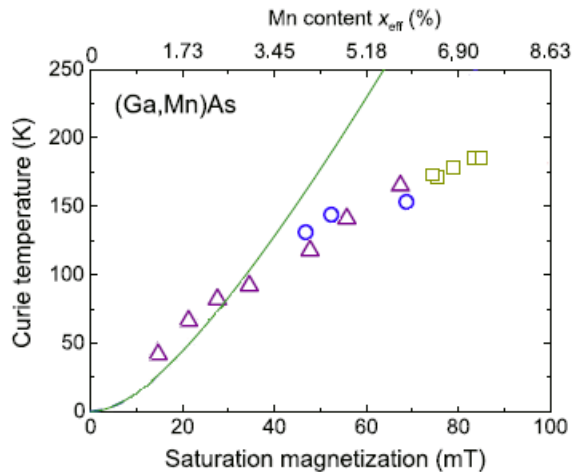


Figure 2. Predicted (green curve) vs. experimental (symbols) Curie temperatures.²

The complete model, known as the p-d Zener model, predicts that the Curie temperature should increase with increasing level of Mn incorporation. Experimental results have confirmed the positive correlation, but show significant deviations from theory at low (<1%) and high (>4%) doping levels (**Figure 2**).^{8,2}

Application of the Zener model to other materials led to the prediction that Mn-doped GaN, InN, and ZnO should exhibit Curie temperatures above room temperature.⁸ This prediction generated enormous interest in these materials, but a reliable conclusion about the actual properties of these materials remains elusive.^{6,9} The attainable Curie temperatures in bona fide Mn-doped GaN samples are far lower than those predicted by the p-d Zener model.²

An alternative approach to understanding the factors that govern the Curie temperatures in DMSs uses a molecular orbital model involving one-electron MOs, combined with *ab initio* calculations. Coupling between the spins of the hole and the Mn centers is maximized by increasing orbital overlap between Mn 3d-orbitals and the semiconductor host donor orbitals (**Figure 3**). The shorter bond lengths in GaN compared to those in GaAs result in increased spin coupling, leading to the original prediction of high Curie temperature. However, increased orbital overlap will also elevate the acceptor orbitals to an energy level well above the valence band maximum of the semiconductor host, making the holes more localized and reducing the spatial range of ferromagnetic interaction (**Figure 3**).^{10,2}

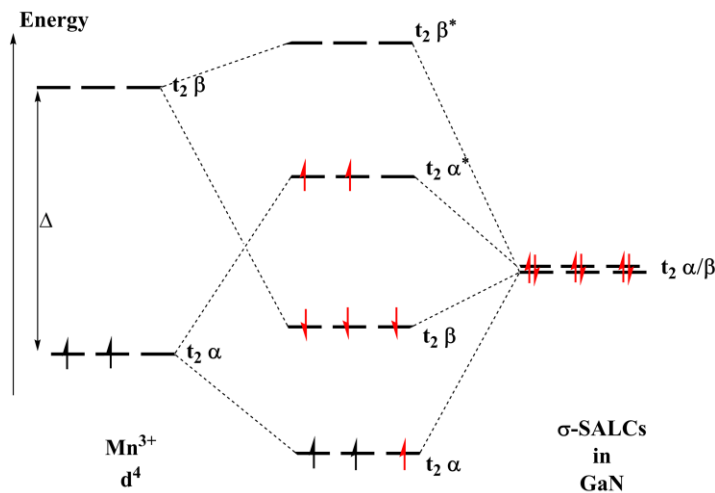


Figure 3. One-electron MO description of Mn-doped GaN.

Further research in this field would likely involve a) continued exploration of device concepts using Mn-doped III-V semiconductors, b) application of characterization techniques that are better able to determine the factors that affect the Curie temperatures, and c) exploration of other structural classes that may exhibit carrier-mediated ferromagnetism.^{6,2}

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