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Transition from Ferromagnetism to Antiferromagnetism in $\mathbf{Ga_{1-x}Mn_xN}$ GUSTAVO DALPIAN, SU-HUAI WEI, National Renewable Energy Laboratory — $Ga_{1-x}Mn_xN$ has attracted much attention recently because previous theoretical predictions suggested that it has a ferromagnetic (FM) ground state with T_c above the room temperature. However, available experimental data often contradict each other. Some reports show that high T_c FM phase is achievable in GaMnN; others show that the magnetic coupling of the Mn ions in GaMnN is actually antiferromagnetic (AFM). The exact nature of the magnetism observed in this system is also under debate. To help unravel the magnetic properties of this system, we developed a new band-coupling model to show that FM order in this system is facilitated by coupling between occupied majority d states inside the gap, whereas AFM ordering in this system is caused by coupling between majority spin d band and minority spin *d* band. At low Mn concentration $Ga_{1-x}Mn_xN$ is FM, whereas at high Mn concentration, under pressure, or if the hole at the Mn *d* band is compensated, $Ga_{1-x}Mn_xN$ will change to AFM ground state. Our *ab initio* total energy calculation based on spin density functional theory support this model.

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