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Effect of Fermi level on Microstructure and Magnetism in (Ga,Mn)N Alloys[1] JENNIFER CHAN, ZHE LIU, STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — GaN doped with Mn has been shown experimentally to exhibit either ferro- or antiferro- magnetic behavior, the results varying considerably depending on the microstructure of the sample. Indeed, the electronic structure and magnetic properties appear to be heavily dependent upon growth conditions and ordering of the material. We used *ab-initio* calculations to investigate the magnetism of various ordered structures of (Ga,Mn)N with respect to Mn composition. The results show that high-spin states with the spins on the Mn aligned in parallel (HS-FM) are stable at low Mn composition (<0.5%) but not at high Mn composition (>0.5%). Instead, for high Mn composition, low-spin states (LS-FM) or states where the spins on the Mn are antiparallel (FI) are found. Interestingly, upon raising the Fermi level, the HS-FM states are stable for all Mn compositions and their formation enthalpies lower with respect to the neutral Fermi level case indicating that electron doping leads to enhanced Mn solubility and hence charged microstructure. The short and long range ordering, tendency for clustering and magnetic properties will be investigated.

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