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Calculation study of Curie Temperature in GaAs based diluted magnetic semiconductor JIALEI XU, Arizona State University, MARK VAN SCHILFGAARDE, Arizona State University, GERMAN D. SAMOLYUK, Ames Laboratory, Iowa State University — We present calculations study of several attempts to increase the Curie Temperature in Mn doped GaAs. In our calculation, the local spin density approximation is combined with a linear-response technique to map the magnetic energy onto a Heisenberg hamiltonion, but no significant further approximations are made. Special quasi-random structures in large unit cells are used to accurately model the disorder. Tc is computed using cluster variation method developed for the classical Heisenberg model. By artificially changing the Fermi level of Mn:GaAs, our calculation indicated the Tc of this system can reach its maximum with half filled band. This result shows a similar picture with double exchange model. This effect was also confirmed by using a virtual dopant with atomic number between Mn and Cr. This result suggests a route to increase Tc by co-doping of Mn and Cr in GaAs. However, our calculation for the disordered Mn and Cr co-doped GaAs shows the decrease in Tc, which may be due to the charge transfer from Cr into Mn. We also investigate the delta-doped Mn:GaAs. By study the different configuration and doping concentration. We found the Tc of one delta-layer structure can reach its maximum with moderate doping concentration ($\sim$25% in the layer).

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