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First-Principle Calculation of The Effective Hamiltonian for (Ga,Mn)As and (Ga,Mn)N RYKY NELSON, ANH NGO, Louisiana State University, WEI KU, Brookhaven National Laboratory, JUANA MORENO, MARK JARRELL, Louisiana State University — Most of the models used to study (Ga,Mn)As have failed to explain the experimental results of (Ga,Mn)N especially its ferromagnetic critical temperature T_c. The need for a consistent and comprehensive model for the dilute magnetic semiconductors (DMS) motivates our study. We obtain the effective Hamiltonian for (Ga,Mn)As and (Ga,Mn)N using a Wannier function based first-principles method. We use density functional theory to calculate the band structure of a range of disordered supercell configurations of (Ga,Mn)As and (Ga,Mn)N and Wannier functions to obtain downfolded Hamiltonians. Those are then disorder averaged to get an effective Hamiltonian. We solved this effective model using the dynamical mean field approximation.

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