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Microscopic Hamiltonian for dilute magnetic semiconductors YUCEL YILDIRIM, ORNL, UT, FSU, ADRIANA MOREO, ORNL, UT, GONZALO ALVAREZ, ORNL, ELBIO DAGOTTO, ORNL, UT — We formulated a real space Hamiltonian to study the effect of dilute magnetic doping of III-V semiconductors. A p-type valence band is considered and nearest neighbor hopping of holes in a diamond lattice is allowed. The relevant hopping parameters between orbitals are obtained using the Slater technique. Considering the effects of the spin-orbit interactions the number of degrees of freedom per site is reduced from 6 (3 orbitals and two spin orientations for the p bands) to 4 (the four projections corresponding to j=3/2 which is the quantum number of the heavy and light hole bands). The ferromagnetic interaction between the doped magnetic impurities and the spin of the mobile holes is written in the appropriated base. The numerical values of the hopping parameters and Hund interaction are obtained from the literature for the different compounds and, thus, there are no free parameters. The properties of the materials are calculated using numerical techniques. The newly developed TPEM method allows us to consider lattices as big as 6x6x6 cubes containing 8 ions each. Finite size effects are very small when systems larger than 3x3x3 cubes are considered. For Mn doped GaAs we reproduce the experimentally observed Curie temperatures for all the studied values of effective hole dopings. For Mn doped GaN our results predict above room temperature Tc's.

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