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Numerical Study of Magnetically doped III-V Zinc-Blende-Type Semiconductors YUCEL YILDIRIM, FSU, ORNL, UT, GONZALO ALVAREZ, ORNL, ADRIANA MOREO, ORNL, UT — Using a newly developed real-space Hamiltonian for zinc-blende dilute magnetic III-V semiconductors we study the properties of a variety of materials. The hopping parameters are functions of the tabulated Luttinger parameters of the III-V parent compounds, and the dispersion of the heavy-hole, light-hole, and split-off bands is reproduced next to the top of the valence band in the undoped case. The exchange interaction parameter J is obtained from measurements; thus, there are no free parameters in the model. The spin-orbit interaction is considered as well as the randomness in the doping. Unbiased Monte Carlo techniques are applied to clusters containing about 300 III-type ions. After successfully reproducing experimental results for (Ga,Mn)As [1], here we present a comprehensive study of the magnetization vs. temperature, the density of states, and the charge distribution for Mn doped GaSb, GaP, GaN, AlP, and InAs. We also present the calculated Curie temperatures for a variety of Mn concentrations and hole compensations.

[1] Y. Yildirim, G. Alvarez, A. Moreo, and E. Dagotto, preprint October 2006

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