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Large-Scale Monte Carlo Study of a Realistic Lattice Model for $Ga_{1-x}Mn_xAs$[1]

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The properties of Mn-doped GaAs are studied at several doping levels and hole compensations, using a real-space Hamiltonian on an fcc lattice that reproduces the valence bands of undoped GaAs. Large-scale Monte Carlo (MC) simulations on a Cray XT3 supercomputer, using up to a thousand nodes, were needed to make this effort possible. Our analysis includes both the spin-orbit interaction and the random distribution of the Mn ions. The hopping amplitudes are functions of the GaAs Luttinger parameters. At the coupling exchange $J{\sim}1.2$ eV deduced from photoemission experiments, the MC Curie temperature and the shape of the magnetization curves are in good agreement with experimental results for annealed samples. The system is found to be qualitatively closer to a hole-fluid regime than to localized carriers. The methodology described here introduces a quantitative tool to analyze a variety of diluted magnetic semiconductors, valid in broad regimes of parameter space.

[1]Y. Yildirim, G. Alvarez, A. Moreo, and E. Dagotto, preprint, October (2006). Supported by DE-AC05-000R22725, DMR-0443144 and DMR-0454504.