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GdN: an excellent candidate for high performance spintronic devices CHUN-GANG DUAN, R.F. SABIRYANOV, W.N. MEI, Dept. of Physics, University of Nebraska at Omaha — We report a detailed theoretical study of the electronic structure and magnetic properties of GdN. Based on first-principles total energy calculations, we deduced the exchange interaction parameters of GdN from fitting the total energies of different magnetic configurations to those computed from the Heisenberg model. The Curie temperature obtained by the Monte Carlo simulation agreed well with experiment. Furthermore, we found strong lattice constant dependence of the exchange parameters of GdN. Our band-structure analysis provides a convincing explanation to this phenomenon. In addition, from the band structures studies of the spin majority and minority of GdN, we expect this compound, which is an excellent half-metallic ferromagnet with a large half-metallic gap, could be utilized for spintronics devices.

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