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Rare-earth nitrides: an LSDA+U study PAUL LARSON, WALTER LAMBRECHT, Case Western Reserve University, MARK VAN SCHILFGAARDE, Arizona State University — The class of rare-earth (Ce-Lu) nitrides all form in the rocksalt crystal structure. One member in particular, GdN, has received considerable theoretical and experimental interest because it appears to be a bulk ferromagnetic semiconductor. The other members of this class of compounds have received much less attention. Electronic structure calculations for the entire series are presented here using a full-potential linear muffin-tin orbital (FP-LMTO) method within the LSDA+U approach. In this approach the localized orbitals have their Coulomb interactions treated in a screened Hartree-Fock mean field approximation while the remaining orbitals are treated in the standard local spin density approximation. U terms were also added to the rare-earth $5d$ states to correct for the underestimation of the band gap in LSDA. In a cubic field, the $4f$ states split into triply degenerate t_{1u} and t_{2u} states and a singly degenerate a_{2u} state. The large Hubbard U is found to dominate crystal field splitting to determine the order of minority and majority spins. Avoiding partially filled states at the Fermi level is the dominant principle, yielding narrow gap semiconducting or semimetallic band structures. In a few cases, namely those which correspond to configurations deviating by 2 electrons from a completely empty, completely full, or half-full configuration, however, an f-band is forced to cross the Fermi level, possibly resulting in heavy-fermion metallic behavior.

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