ScN:Mn a dilute ferromagnetic semiconductor ADITI HERWAD-KAR, WALTER R. L. LAMBRECHT, Dept. of Physics, Case Western Reserve University, Cleveland OH 44106 — We study the electronic properties of ScN:Mn calculated using the full potential linearized muffin-tin orbital method. To model the impurity we use 64 atom supercells and fully relax the structure. Band gap corrections are included in a closely related atomic sphere approximation (ASA). Mn on a Sc site is found to induce a localized state in the middle of the band gap of ScN with t_{2g} character. Its spin splitting leads to a net magnetic moment of 2-3 μ_B per Mn. Calculations of unit cell for near neighbor Mn atoms reveal that the spins prefer ferromagnetic coupling. Using mean field approximation and assuming a random distribution of Mn atoms we estimate the Curie temperature. Above room temperature T_c seems possible with only 2 % Mn concentration. The Gibbs energy of formation of the Mn impurity is found to be 3.6 eV, which is comparable to that of other magnetic semiconductor systems. The shared rocksalt structure of MnN and ScN should facilitate alloy formation. The energy of formation of the Mn pairs indicates, no tendency towards clustering. Notably, the ferromagnetic coupling in this system occurs even without the condiseration of a carrier mediated coupling mechanism. The presence of local magnetic moments on Mn results in a small spin splitting of the Sc d-like conduction bands, so one could expect to see interesting effects on carrier transport in n-type ScN:Mn. A high n-type concentration however may tend to reduce the magnetic moments.

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