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Exchange interactions in Mn-doped ScN ADITI HERWADKAR, Case Westrn Reserve University, WALTER R. L. LAMBRECHT , Case Western Reserve University — We present a computational study of the exchange interactions in Mn-doped ScN. First, we test to what extent the Heisenberg Hamiltonian applies to large spin rotations. We calculate them instead from a non-collinear calculation with a small rotation. This shows that the exchange interactions obtained from a collinear energy difference (antiferromagnetic- ferromagnetic) would be overestimated by about 30%. Next, we calculate the exchange interactions using the linear response multiple scattering theory approach of Liechtenstein et al. We find $\sum_j J_{0j}$ for a nearest neighbor pair is the same as before, but we now find this to be a sum over many long-range interactions. The actual near neighbor interactions are an order of magnitude smaller. Finally, we study various special quasirandom structures with 256 and 432 atoms per cell with concentrations of 3-10 %. These calculations indicate that with randomness, many of the long-range interactions become negative and thus lead us to believe that Mn-doped ScN is not a ferromagnetic semiconductor but a spin-glass. These calculations do not yet include the effects of n-type doping,which might add ferromagnetic couplings for long-range neighbors.

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