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Ferromagnetism in GdN: an antiferromagnet in disguise. WALTER R. L. LAMBRECHT, CHANDRIMA MITRA, Case Western Reserve University — We analyze the exchange interactions in GdN and Gd pnictides GdX with X=P,As,Sb,Bi using full-potential linearized muffin-tin orbital calculations as well as the linear response approach in the atomic sphere approximation. We show that in GdN, the ferromagnetism arises from the small induced opposite magnetic moments on Gd-d and N-p orbitals. When these form a perfect antiferromagnetic arrangement on the rocksalt lattice, it pins the large magnetic 4f moments in a ferromagnetic arrangement through the on-site f-d coupling. In contrast, in the other pnictides, the AFM-II (111)-ordered state is preferred, in which case there is no moment induced on N. The Néel temperatures as well as the Curie-Weiss temperatures extracted from this model are in good agreement with experiment for the pnictides, but the Curie temperature of GdN in this model is only about 10 K, strongly underestimating the experimentally observed Curie temperature of about 70 K. Linear response calculations give an alternative view including exchange interactions with empty spheres but give consistent estimates of T_c and also give a reasonable Curie temperature for metallic Gd. We find that adding n-type doping by shifting the Fermi level does not increase T_c in GdN substantially but adding N-vacancies explicitly does. Thus, it seems that defects play a significant role in establishing the Curie temperature of GdN.

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