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Defect induced ferromagnetism in Gd doped GaN CHANDRIMA MITRA, WALTER LAMBRECHT, Case Western Reserve University — We review various suggested mechanisms for the ferromagnetism in Gd-doped GaN using local spin density approximation supercell calculations. The spin splitting of the conduction band induced by the Gd $s-f$ coupling is found to decrease linearly with Gd concentration and hence colossal magnetic moments cannot be explained by filling this spin-split band with ionized donor electrons. Furthermore we find the Gd-Gd interactions to be antiferromagnetic except in p-type material. Although, Ga vacancies can induce long range interactions and up to three Bohr magneton moments per vacancy in the neutral charge state, we note that these defects only are favorable to form in n-type materials and then should predominantly occur in a 3− charge state which has no magnetic moment. N-interstitials are likely to form in conjunction with N vacancies for mid gap Fermi levels consistent with the semi-insulating nature of the samples and have a magnetic moment for the corresponding charge state. We find that Gd in the presence of N interstitials alone prefer antiferromagnetic coupling but in the presend of both N-interstitials and N vacancies prefer ferromagnetic coupling. We find that oxygen tends to seggregate toward an interstitial site near the Gd and in that case can induce a strong ferromagnetic coupling between Gd.

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