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Electronic structure of Gd impurities in GaN on Ga, N and Ga-N adjacent sites and the role of N interstitials TAWINAN CHEIWCHANCHAMNANGIJ, WALTER LAMBRECHT, Case Western Reserve University — Gd-doped GaN is one of the most interesting dilute magnetic semiconductors. However, the origins of its magnetic properties are still unclear. Previous studies have focused on the role of intrinsic defects, such as Ga vacancies and N or O interstitials. Here, we study Gd doped in pairs on adjacent Ga and N sites, which were suggested to be required to explain the X-ray linear dichroism signals in Gd L-edge spectra by Ney et al. JMMM 322, 1162 (2010). By using the FP-LMTO method in the LSDA+U, we find that the Gd on N site is pushed to the interstitial site after the relaxation and there is no extra magnetic moment besides the seven Bohr magneton from the 4f half-filled shell on each Gd atom. In spite of the relaxation, we find the energy of formation of this cluster to be of order 10 eV, which shows that the Gd doped on Ga-N adjacent sites is unlikely to occur. We also study Gd doped on a single N site and find an excess magnetic moment of 3 Bohr magneton which is spread over Gd, the nearest neighbor Ga atoms, and second nearest neighbor N atoms. However, its energy of formation is also large that this kind of impurity is unlikely to occur. We critically examine previous work on the role of N interstitials in the magnetism of Gd-doped GaN by studying the magnetic properties of the split interstitials, their interaction with each other and with Gd.

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