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Calculated x-ray linear dichroism spectra for Gd-doped GaN TAWINAN CHEIWCHANCHAMNANGIJ, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University — Gd doped GaN has been claimed to be a dilute magnetic semiconductor with colossal magnetic moments. However, the origin of huge magnetic moments is still controversial. The x-ray linear dichroism (XLD) spectrum of the Gd L3 edge and the multiple scattering calculations from Ney et al. (J. Magn. Magn. Mater. 322, 1162 (2010)) suggested that about 15% of Gd atoms should be on antisites. In contrast, our first principle calculations indicate that once the Gd is put on the N site, it will move to the interstitial site and cause large structure relaxation. The formation energy of the system is, therefore, in the order of 10 eV per Gd atom which is extremely large. We show that XLD spectra for L-edges can be analyzed in terms of suitable linear combinations of the partial densities of states of the Gd d-electrons. Core-hole effects are also included. The XLD spectra extracted from our calculations of Gd on the Ga site is shown to fit the experimental spectrum and no Gd on the N site is needed.

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