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Role of nitrogen vacancies and related complexes in compensation and luminescence of Mg-doped GaN QIMIN YAN, ANDERSON JANOTTI, University of California at Santa Barbara, MATTHIAS SCHEFFLER, UCSB and Fritz-Haber-Institut, D-14195 Berlin, CHRIS G. VAN DE WALLE, University of California at Santa Barbara — Using first-principles calculations with the hybrid functional method (HSE), we investigate the effects of nitrogen vacancies and related complexes on the electrical and optical properties of Mg-doped GaN. We obtain information about the expected defect concentration, stable charge states, and defect levels by calculating the formation energies of vacancies and Mg−vacancy complexes. The 3+ state of the nitrogen vacancy and the 2+ state of the complex are found to be most stable when the Fermi level is near the valence-band maximum (VBM). Our calculations also enable us to study the role of these defects in luminescence. Vacancy-dopant complexes (including Mg_{Ga}−V_N) have been proposed as the origin of a deep level involved in the red (1.8 eV) photoluminescence (PL) band often observed in Mg−doped GaN. We investigate the optical absorption and emission energies by calculating the configuration coordinate diagram for the vacancy and for the Mg_{Ga}−V_N complex. The emission, in which an electron in the conduction band is transferred to $(Mg_{Ga}-V_N)^{2+}$, resulting in $(Mg_{Ga}-V_N)^{+}$, peaks at 1.81 eV. Our calculated emission lines thus indicate that Mg_{Ga}−V_N is a likely source for the red luminescence observed in Mg-doped GaN.

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