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Carbon Defect Complex as a Source of Yellow Luminescence in GaN DENIS DEMCHENKO, MIKHAIL RESHCHIKOV, Virginia Commonwealth University — Using hybrid functional theory compared with experimental measurements, we demonstrate that yellow luminescence often observed in both carbon-doped and pristine GaN is the result of electronic transitions via C_N-O_N complex. In contrast to the common isolated defects, C_N-O_N complex is energetically favorable, and its calculated optical properties as well as the thermodynamic transition level show excellent agreement with the measured luminescence data. Calculated transitions via the localized defect states of this complex are (experimental values are given in brackets): thermodynamic transition level of 0.75 eV (0.85 eV), absorption energy 3.30 eV (3.32 eV), emission energy 2.25 eV (2.20 eV), and zero phonon transition 2.70 eV (2.60 eV). This complex has not been proposed as a source of the yellow band in GaN, while all other defects previously suggested to be sources of this band exhibit high formation energies and would produce red or infrared photoluminescence. Thus, combining hybrid density functional theory and experimental measurements we propose a solution to a long-standing problem of the GaN yellow luminescence.

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