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Mg acceptors and the ultraviolet band in Mg-doped GaN.¹ IBRAHIMA DIALLO, DENIS DEMCHENKO, MICHAEL RESHCHIKOV, Virginia Commonwealth Univ — The sharp ultraviolet luminescence (UVL) band with a maximum photoluminescence and zero-phonon line at approximately 3.25-3.30 eV is observed in magnesium (Mg) doped GaN. Using the hybrid density functional method, we calculate electronic and optical properties of Mg acceptors in GaN. We show that Mg substituting Ga is responsible for the experimentally observed sharp UVL band in Mg-doped GaN. We also analyze the dual nature of Mg acceptors in GaN.

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