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Hybrid functional calculations of DX centers in AlN, GaN and AlGaN[1] LUKE GORDON, JOHN L. LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — The group-III nitrides have important commercial applications in optoelectronic devices. To achieve high-efficiency UV lasers and LEDs, AlN substrates and high Al-content AlGaN alloys will likely be required. A better understanding of the role of defects and impurities in AlN is crucial. One of the outstanding problems in the study of AlN and high-Al-content AlGaN is the formation of the so-called DX centers, which consist of donor impurities that self-compensate by turning to acceptors as the Fermi level approaches the conduction band. In this work, we employ density functional calculations using a hybrid functional to investigate the possibility of DX-center formation for Si and O donors in AlN and GaN. The functional includes a portion of Fock exchange and gives band gaps and lattice parameters very close to the experimental values, allowing for quantitative predictions of defect levels. Based on the analysis of the stability of DX centers in AlN and GaN, we discuss the onset of DX behavior in AlGaN alloys.

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