

Abstract Submitted
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Reconstructions and adsorbates on polar and nonpolar GaN surfaces DAVID SEGEV, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Recently, exciting progress has been made in the ability to grow GaN in nonpolar orientations. We report on a systematic study of the reconstructed GaN *a* (1120), *m* (1010) and *c* (0001) planes. Using first-principles calculations, based on density-functional theory within the local density approximation (LDA), we examine the structural and electronic dissimilarities between the polar and the nonpolar surfaces. Adatom energetics and doping issues have been also investigated for the different surfaces considered. We propose a simple way to overcome the band-gap underestimation problem inherent in density-functional theory. New features will be presented, in light of the available experimental data.

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