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Identifying microscopic mechanisms for hole traps in nitride heterostructures[1] JOHN LYONS, LUKE GORDON, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Some recent designs of nitride semiconductor devices employ heterostructures (such as N-face high-electron-mobility transistors) in which the electronic Fermi level is established near the valence-band maximum due to the influence of polarization fields. In many of these heterostructures, the presence of hole-trapping centers is thought to adversely affect device performance. This behavior has been observed in many different types of devices, and its physical origin remains unknown. Using first-principles calculations based on a hybrid functional, we investigate possible origins for this phenomenon. We explore both intrinsic defect candidates as well as impurities. With Schrödinger-Poisson simulations, we then investigate how the behavior of these species and their spatial distribution within the heterostructure layers is reflected in the performance of nitride semiconductor devices.

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