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Electronic structure of nitride surfaces CHRIS G. VAN DE WALLE, DAVID SEGEV, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara, California 93106, USA — Knowledge of surface reconstructions and the corresponding surface electronic structure is important to control growth, since Fermi-level pinning can affect defect creation and incorporation. In addition, surface states can play an important role in devices, for instance in high-electron mobility transistors where the surface acts as a source of electrons for the channel. In the case of InN a very high, and thus far unexplained, electron accumulation has been observed on all polar surfaces. We have addressed these issues by performing a systematic computational study of reconstructed GaN and InN surfaces in various orientations, including (11-20) (a plane) and (10-10) (m plane), as well as the polar (0001) ($+c$) and (000-1) ($-c$) planes. The calculations are based on density-functional theory, combined with an extensively tested approach for correcting the band-gap error through use of modified pseudopotentials. For GaN we identify the microscopic origins of the experimentally observed Fermi-level pinning. For InN we find that on polar surfaces occupied surface states occur above the conduction-band minimum, thus explaining the observed electron accumulation. We predict an absence of electron accumulation on *nonpolar* surfaces grown at moderate In/N ratios.

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