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Theoretical Analysis of the Band Offsets and Band Bending in (0001) $In_xGa_{1-x}N$/GaN Heterostructures and Quantum Wells LIANG DONG, Department of Physics, University of Connecticut, S. PAMIR ALPAY, Department of Physics and Institute of Materials Science, University of Connecticut — Valence band offsets (ΔE_V) and built-in electric fields of (0001) $In_xGa_{1-x}N$/GaN heterostructures and quantum wells are studied as a function of In composition x using first principles calculations based on density functional theory (DFT). These properties determine the degree of quantum confinements and wave function overlapping of electrons and holes, and thus the overall efficiencies of electronic/optoelectronic devices based on these structures. We show that with increasing x, ΔE_V of (0001) $In_xGa_{1-x}N$/GaN displays a parabolic bowing in both strain-free (fully relaxed) heterostructures and pseudomorphic quantum wells on c-plane GaN substrates. ΔE_V of (0001) InN/GaN in these two cases (0.98 eV and 0.64 eV, respectively) can be used to explain the deviations in experimental results that vary from 1.1 eV to 0.58 eV. We also show that the DFT calculated built-in electric fields in these constructs agree with continuum-level electrostatic analysis based on Maxwell and Poisson's relations, taking into account the first and second order of piezoelectric couplings.

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