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Strain effect in group-III nitride semiconductors and their alloys QIMIN YAN, PATRICK RINKE, Materials Department, Univ. of California, Santa Barbara, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, CHRIS VAN DE WALLE, Materials Department, Univ. of California, Santa Barbara — Strain plays a crucial role in group-III nitride semiconductor based devices since it affects the band structure near the valence- and conduction-band edges and thus the optical properties and the device characteristics. However, the deformation potentials that describe the change in band structure under strain have not yet been reliably determined. We present a systematic study of the strain effects in AlN, GaN and InN in the wurtzite phase. We apply density functional theory and hybrid functionals to address the band-gap problem. We observe nonlinearities of transition energies under realistic strain condition that may, in part, explain the appreciable scatter in previous theoretical work on deformation potentials of group-III-nitrides. For the linear regime around the experimental lattice parameters, we present a complete set of deformation potentials. Applying our deformation potentials, we study strain effects in InGaN alloys (including c-, m-, and semi-polar planes) grown on GaN substrates. We make predictions for the transition energies in these systems and their dependence on In composition.

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