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Band Gap Tuning and Structural Transformation in GaN through Equi-biaxial In-plane Strains and Alloying with InN LIANG DONG, Department of Physics, University of Connecticut, S. PAMIR ALPAY, Department of Physics and Institute of Materials Science, University of Connecticut — Gallium nitride (GaN)-based semiconductor devices play a key role in modern optoelectronics and photovoltaics. Structural and electronic properties of the GaN can be tuned through external/internal stresses or by alloying it with InN. In this study, we present an *ab initio* analysis using density functional theory to understand the effects of equi-biaxial strains and indium additions to the crystallographic structure, electronic properties, and polarization of GaN and band bending in GaN-InN heterostructures. It is shown that internal strains in GaN may result in significant changes in the band gap and may even give rise to structural transformations from wurtzite to a graphite-like semi-metallic phase. For the InGaN alloys, possible stable crystal structures (besides the prototypical wurtzite structure), lattice parameters, the band gap, and the spontaneous polarization are calculated as function of indium composition.

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