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First-Principles determination of deformation potentials in nitrides QIMIN YAN, PATRICK RINKE, MATTHIAS SCHEFFLER, CHRIS G. VAN DE WALLE, University of California at Santa Barbara — Group-III nitrides and their alloys are now commonly used in optoelectronic devices such as light emitting diodes (LEDs) and laser diodes (LDs). In these devices strain plays a crucial role since it affects the band structure near the valence- and conduction-band edge and thus the optical properties and the device characteristics. The deformation potentials that describe the change in band structure under strain have not yet been reliably determined, either experimentally and theoretically. Here we present a systematic study of the strain effects in AlN, GaN and InN in the zinc-blende and wurtzite phase. Besides density functional theory (DFT) in the most commonly applied local- and gradient corrected density approximation (LDA/GGA) we also apply the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional [1] and G_0W_0 quasiparticle corrections to address the band gap problem. We present a complete set of deformation potentials that allows us to predict the band positions under realistic strain conditions. For the wurtzite phase we observe non-linearities in the strain dependence that may, in parts, explain the appreciable scatter in previous theoretical work on deformation potentials of group- III-nitrides. [1] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003) Work supported by the UCSB Solid State Lighting and Energy Center.

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