

Valence Band Effective Hamiltonians in Nitride Semiconductors from QSGW Band Structures

A. Punya and W. R. L. Lambrecht

Department of Physics, Case Western Reserve University, Cleveland, OH 44106, USA.

To determine the electronic states, optical properties and transport in quantum wells, quantum wires and quantum dots of nitride semiconductors, one uses valence band effective Hamiltonians within the effective mass approximation. Although significant experimental and theoretical work has been performed in the past, basic parameters such as the Rashba Sheka Pikus (RSP) Hamiltonian parameters are still uncertain [1]. In the present work, the electronic band structures of wurtzite AlN, GaN and InN as well as the RSP Hamiltonian parameters are determined by using the quasiparticle self-consistent GW (QSGW) approximation [2, 3] in a full-potential linearized muffin tin orbital (FP-LMTO) implementation [4]. The present GW implementation offers more accurate band structures beyond the local density approximation (LDA) since the self-energy is calculated in a real space representation and able to interpolate on arbitrarily fine k-point meshes. Hence, splittings and effective masses can be obtained accurately. We find the crystal field splitting in GaN (12 meV) in much closer agreement with experiment than previous work and obtain a negative spin orbit coupling for InN. Moreover, we have generalized the method of invariants to crystals with orthorhombic symmetry, such as ZnSiN_2 , ZnGeN_2 , ZnSnN_2 and CdGeN_2 and determined the corresponding Hamiltonian parameters. These materials have two different crystal field splittings and several additional effective mass parameters. The spin-orbit splitting parameters in them are found to be negligibly small.

This work is funded by the NSF.

- [1] I. Vurgaftman and J. R. Meyer, J. Appl. Phys. **94**, 3675 (2003).
- [2] M. van Schilfgaarde, T. Kotani, and S. Faleev, Phys. Rev. Lett. **96**, 226 402 (2006).
- [3] T. Kotani, M. van Schilfgaarde, and S. V. Faleev, Phys. Rev. B **76**, 165 106 (2007).
- [4] T. Kotani and M. van Schilfgaarde, Phys. Rev. B **81**, 125 117 (2010).