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Valence band effective Hamiltonians in nitride semiconductors
ATCHARA PUNYA, NUCHAREE SCHWERTFAGER, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106 — Valence band effective Hamiltonians are useful to determine the electronic states of shallow impurities, quantum wells, quantum wires and quantum dots within the effective mass approximation. Although significant experimental and theoretical work has been performed, basic parameters such as the Rashba Sheka Pikus (RSP) Hamiltonian parameters are still uncertain. In this work, the electronic band structures of AlN, GaN and InN, all in the wurtzite crystal structure, as well as the RSP Hamiltonian parameters are determined by using the QSGW approximation in a FP-LMTO implementation. The corrections offered by this approach beyond the LDA are important to obtain the splittings and effective masses accurately. The present GW implementation, which allows for a real space representation of the self-energy, enables us to interpolate exactly to a fine k-mesh and hence to obtain accurate effective masses. We find the crystal field splitting in GaN (12 meV) in much closer agreement with experiment than previous work and obtain a negative SO coupling for InN. Moreover, we have generalized the method of invariants to crystals with orthorombic symmetry, such as $ZnSiN_2$ $ZnGeN_2$, $ZnSnN_2$ and $CdGeN_2$ and determined the corresponding Hamiltonian parameters.

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