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Effective mass calculations for shallow acceptors in nitrides[1] JACOB EMMERT-ARONSON, W.R.L. LAMBRECHT, CWRU — In the effective mass approximation for shallow acceptors in semiconductors, the defect eigenstates are written as a product of a slowly varying envelope function and the band extrema Bloch functions. The Kohn-Luttinger Hamiltonian describing the valence band manifold in zincblende, or its generalization for other crystals structures, then becomes a set of coupled differential equations for the envelope function. These can be solved by a variational approach with hydrogenic type basis functions. We have implemented this approach for the appropriate Hamiltonians for zincblende, wurtzite and an orthorhombic crystal structure occurring for II-IV-N2 semiconductors. The Hamiltonian parameters used were extracted from first-principles GW calculations. The central cell correction to the Coulomb potential was added based on pseudopotential differences as proposed by Mireles and Ulloa (Phys. Rev. B 58, 3879 (1998)). Results are presented for various acceptors in GaN, AlN, InN, ZnGeN2 and ZnSnS2. The effects of varying the crystal field splitting parameter, and the type of pseudopotentials (including or not semicore d-states) were investigated.

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