

Realistic g-factors, effective mass and k.p parameters for III-V semiconductors from 14-band k.p Hamiltonian

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Recently, we developed a procedure to determine effective mass parameters from DFT calculations that provided realistic band structures for $8 \times 8 k \cdot p$ ZB Hamiltonians[1,2]. Although band structures reproduced the other methods up to 20 % of the First Brillouin Zone and the calculated g-factor are in agreement with literature for such Hamiltonians, the g-factors for small band gap materials are not realistic due to the proximity of bands which are not taken into account in the usual $8 \times 8 k \cdot p$ Hamiltonian. In this work we go further in the analysis of the g-factors by analyzing Hamiltonians with different number of states and approximation orders. Our goal is to determine if one can theoretically achieve realistic values also for g-factors by playing with the number of bands of the Hamiltonian using the Roth approximation [3] to a higher order, using also realistic Kane P_1 and Q interband interaction parameters.

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