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Ab-initio Prediction of Conduction Band Spin Splitting in Zincblende Semiconductors ATHANASIOS CHANTIS, MARK VAN SCHILFGAARDE, TAKAO KOTANI, Arizona State University — We use a recently developed self-consistent *GW* approximation to present systematic *ab initio* calculations of the conduction band spin splitting in III-V and II-V zincblende semiconductors. The spin orbit interaction is taken into account as a perturbation to the scalar relativistic Kohn-Sham hamiltonian. These are the first calculations of conduction band spin splittings based on a quasiparticle approach. We show that the self-consistent *GW* scheme accurately reproduces the relevant band parameters, and is therefore expected to be a reliable predictor of spin splittings. The results are compared to the few available experimental data and a previous calculation based on a model one-particle potential. We show that the commonly used $\mathbf{k} \cdot \mathbf{p}$ hamiltonian is missing contributions, and cannot reliably reproduce the splittings.

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