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Full-zone spin-splitting for electrons and holes in bulk GaAs and GaSb[1] JUN-WEI LUO, GABRIEL BESTER, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — The spin-orbit interaction — a fundamental electroweak force — is equivalent to an effective magnetic field intrinsic to crystals, leading to band spin-splitting for certain k-points in sufficiently low-symmetry structures. This (Dresselhause) splitting has usually been calculated at restricted regions in the Brillouin-zone via small-wavevector approximations (e.g., $\mathbf{k} \cdot \mathbf{p}$). We provide a full-zone description of the Dresselhaus splitting in zinc-blende semiconductors by using pseudopotentials, empirically corrected to rectify LDA errors by fitting GW results at a few firections. We find that (i) The largest spin-splitting occurs along the [210] direction, not the [110] direction as previously thought based on limited view of the Brillouin zone; (ii) The spin-splitting of the upper valence band VB1 is comparable to that of the next two valence bands VB2 and VB3. This has been previously overlooked due to the expectation that the largest spin-splitting will occur along the [110] direction; (iii) The spin-splitting pattern of each band is orthogonal to each other.

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