Full-Zone Spin Splitting for Electrons and Holes in Bulk GaAs and GaSb

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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 (Dresselhaus) splitting has usually been calculated at restricted regions in the Brillouin zone via small wave vector approximations (e.g., k p), potentially missing the ''big picture.'' We provide a full-zone description of the Dresselhaus splitting in zinc blende semiconductors by using pseudopotentials, empirically corrected to rectify local density approximation errors by fitting GW results. In contrast to what was previous thought, we find that the largest spin splitting in the lowest conduction band and upper valence band (VB1) occurs surprisingly along the (210) direction, not the (110) direction, and

ously thought, we find that the largest spin splitting in the lowest conduction band (CB1) and upper valence band (VB1) occurs surprisingly along the (210) direction, not the (110) direction, and that the splitting of the VB1 is comparable to that of the next two valence bands VB2 and VB3.

Crystal pseudopotential.—The band structure of bulk material is obtained via direct diagonalization of the single-particle Schrödinger equation in an empirical pseudopotential method (EPM) [15] representation,

$$\left(-\frac{1}{2}\nabla^2 + V(\mathbf{r}) \right)\psi_i(\mathbf{r}) = E_i\psi_i(\mathbf{r}), \quad (2)$$

The crystal potential $V(\mathbf{r}) = \sum_{n,\alpha} v_\alpha(\mathbf{r} - \mathbf{R}_{n,\alpha})$ is a superposition of screened atomic potentials v_α of atom type α located at atomic site $\mathbf{R}_{n,\alpha}$ which contains a local part v_α^L and a nonlocal spin-orbit interaction part $v_{\alpha\ell}$. The nonlocal spin-orbit interaction $v_{\alpha\ell}$ is described by a Kleinman-Bylander separable form [16]

$$v_{\alpha\ell} = \delta_\alpha \sum_{i,j} |i\rangle B(i,j) \langle j|, \quad (3)$$

where i and j are reference functions, and $B(i,j)$ is a matrix representation of the spin-orbit interaction: $B(i,j) = \langle i|\mathbf{L}\cdot\mathbf{S}|j\rangle$, where $\mathbf{L}$ and $\mathbf{S}$ are the spatial angular momentum operator and spin operator, respectively. The pseudopotentials v_α are fitted [17,18] to experimental transition energies, effective masses, and deformation potentials of the bulk material. The supplementary section [18] describes the fit in detail. The wave function $\psi_i(\mathbf{r})$ is expanded by a set of plane waves. Table I gives the critical properties calculated by our standard empirical pseudopotential (EP-I) used previously [14,17]. Although this potential was not fit to the spin splitting, it gives a good representation of the GW results [Fig. 1(a)]. In fact, writing $\Delta_{so}(k) = \Delta_c\, k^2$ we get from our standard EP-I $\Delta_c = 1.3$ eV (Δ_c is in eV Å^2) whereas GW [6] gives $\Delta_c = 1.7$ eV, a big improvement over LDA [21] that gives $\Delta_c = 0.7$ eV [Fig. 1(c)]. Over the full extent of the data shown in Fig. 1, the agreement between LDA and GW is qualitatively good, except near Γ. Indeed, LDA is known to fail for band gaps and for effective masses more dramatically near Γ than in other regions in the zone (see Ref. [6]). Experimental values are indirect and somewhat scattered and are 9.0 [20], 11.0 [20], and 17–35 [20].

It is possible to further improve EP-I [see black line in Fig. 1(b)]. Analysis of the spin splitting [5] reveals that it depends on (1) the energy splittings due to spin-orbit interaction [e.g., $\Delta_0 = E_{\Gamma_{15}^v} - E_{\Gamma_{25'}^v}$, $\Delta_0' = E_{\Gamma_{15}^c} - E_{\Gamma_2^c}$, and $\Delta_1 = \langle E_{L_3^v}|L_z|E_{L_3^v}\rangle$], (2) the position of the two lowest-lying conduction band levels at Γ [i.e., $E_0 = E_{\Gamma_1^c} - E_{\Gamma_{15}^v}$ and $E_0' = E_{\Gamma_{25'}^c} - E_{\Gamma_{15}^v}$], and (3) on matrix elements of the momentum operator and

GaAs pseudopotential (EP-II) gives results described in Table I and Fig. 1(b). It accurately reproduces band energies, effective masses, and spin splitting. It is obvious from the discussion above that two pseudopotentials (EP-I and EP-II) with equally good fit to energy eigenvalues can give different spin splitting if the underlying momentum and spin-orbit matrix elements are different. This suggests that the small-k behavior of $\lambda_i k$ is rather sensitive to the details of the wave functions. Once the crystal potential $V r$ (EP-II) is constructed, we employ it to take a glimpse at the full-zone spin splitting which was not observed before.

Small-k behavior.—The fitted k-cubic terms of small-k spin splitting at the three lowest conduction bands (denoted CB1, CB2, and CB3) and the three highest valence bands (denoted VB1, VB2, and VB3) are given in Table I. Near , VB1, VB2, and VB3 are usually called, respectively, heavy

we can ascertain that the VB1 and CB1 have largest splitting along (210), not along the (110) direction. If we compare the spin splitting of different bands only along the (110) direction, we would have reached an incorrect conclusion that the spin splitting of VB1 is much smaller than VB2 and VB3. From Figs. 2(c) and 3(d)–3(f), however, we can see that the maximal spin splitting of VB1 is actually comparable to that of VB2 and VB3.

Summary.—We have performed full-zone spin splitting calculations of GaAs and GaSb. We find that (i) the largest spin splitting in the CB1 and VB1 occurs along the (210) direction, not the (110) direction that was previous 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 interband coupling significantly influences the spin splitting of related bands. To validate our most surprising EPM result—that the spin splitting has a maximum at another area in the Brillouin zone than previously suspected—we performed an independent test, using self-consistent LDA. Our EPM conclusions were corroborated by LDA. For example, LDA predicts that the maximum spin splitting of GaAs CB1 and VB1 along the (210) direction is 140 and 144 meV; however, along the (110) direction it is only 60 and 8 meV, respectively.

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