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Spin-Orbit Interaction Effects in Zincblende Semiconductors: *Ab Initio* Pseudopotential Calculations

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Spin-Orbit Interaction Effects in Zincblende Semiconductors: Ab Initio Pseudopotential Calculations

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Ab initio band structure calculations have been performed for the spin-orbit interaction effects at the top of the valence bands for GaAs and InSb. Relativistic, norm-conserving pseudopotentials are used with no correction made for the gaps from the local density approximation. The spin-orbit splitting at Γ and linear terms in the $\vec{k}$ dependence of the splitting are found to be in excellent agreement with existing experiments and previous theoretical results. The effective mass and the cubic splitting terms are also examined.

We report results from an *ab initio* calculation of the effect of spin-orbit interaction at the top of the valence bands for GaAs and InSb. The method employed is an extension of the analysis of Hybertsen and Louie [1] to systems without inversion symmetry. In this approach, the relativistic pseudopotentials [2,3] are first used to obtain a scalar relativistic band structure in a planewave local density functional (LDA) calculation, yielding both the unsplit eigenvalues and wavefunctions. The spin-orbit interaction is then added as a perturbation on the self-consistent scalar bands, and the fully relativistic eigenvalues and wavefunctions are obtained at each $\vec{k}$ by diagonalizing the Hamiltonian matrix in the basis of the scalar relativistic wavefunctions. In a planewave basis the perturbation Hamiltonian is given by:

$$H^{so}_{\vec{s},\vec{K};\vec{s}',\vec{K}'} = -i < s|\ \vec{S}\ |s'> \frac{\vec{K}\times\vec{K}'}{KK'} \sum_{n=1,2} e^{i(\vec{K}-\vec{K}')\cdot\vec{\tau}_n}$$

$$\times\{12\pi V^{so,n}_{l=1}(\vec{K},\vec{K}') + 60\pi \frac{\vec{K}\cdot\vec{K}'}{KK'} V^{so,n}_{l=2}(\vec{K},\vec{K}')\} \qquad (1)$$

The notation is equivalent to that in Ref. 1, except that here the basis $\vec{\tau}_n$ yields complex structure factors.

The scalar bands are calculated with a planewave basis extending up to a kinetic energy of 16 Ry for GaAs and 14 Ry for InSb. The calculated LDA direct gaps are 0.485 eV for GaAs and -0.201 eV for InSb without spin-orbit splitting. The spin-orbit perturbation is included for the first 8 scalar relativistic bands (4 valence and 4 conduction). Essentially the same results are obtained near Γ if only the top 3 valence and lowest conduction band are included. The $E(\vec{k})$ are then fitted in the vicinity of Γ for the valence states Γ_7 and Γ_8 to Mth order polynomials in each of the high symmetry directions Δ, Λ, Σ (M is typically 20). The results are summarized in Fig. 1 and Tables 1 and 2 and discussed below:

1) The spin-orbit splitting between the states Γ_7 and Γ_8 are in excellent agreement with experimental results for GaAs and good agreement with experimental InSb results.

2) The linear spin-orbit splittings which arise from the lack of inversion symmetry are precisely consistent with the group theoretical relations in Ref. 4 which have the ratios for different $\vec{k}$ directions (Fig. 1):

$$\frac{C^1_{\Sigma a}}{\sqrt{1+\frac{\sqrt{3}}{2}}} = \frac{C^1_{\Sigma b}}{\sqrt{1-\frac{\sqrt{3}}{2}}} = \frac{C^1_{\Lambda a}}{\sqrt{2}} = C^1_{\Delta ab} = C^1 \qquad (2)$$

$$C^1_{\Lambda bc} = 0 \; ; \quad -C^1_{\Delta cd} = C^1_{\Delta ab} \; ; \quad -C^1_{\Sigma d} = C^1_{\Sigma a} \; ; \quad -C^1_{\Sigma c} = C^1_{\Sigma b} \qquad (3)$$

where C^1 is the linear splitting coefficient in the [100] direction [4,5]. The only available experimental data for InSb is in very good agreement with our calculation. In addition, our results for GaAs are in close agreement with the LMTO calculation of Cardona *et. al.* [6]. This agreement comes despite the small calculated LDA direct gaps. These results indicate that the valence band linear terms are mainly due to the interaction among the Γ_{15} valence bands.

3) The quadratic coefficients and cubic splittings for the Γ_8 bands are listed in Table 2. The quadratic coefficients are strongly anisotropic due, in part, to a mixing of the light and heavy holes in the [100] and [110] directions. The cubic coefficients differ from those of Ref. 6 by two or three orders of magnitude, since the region examined here is close to Γ, so that the light and heavy holes are nearly degenerate and intermix. This is in contrast to Ref. 6, where the analysis was performed for a larger region of $\vec{k}$, so the holes are split by their different effective

masses and do not mix. Additionally, the LDA gaps have not been empirically corrected to the experimental values here.

4) The split-off hole band is very isotropic and parabolic with quadratic coefficients of -37 eVÅ^2 for GaAs and -91 eVÅ^2 for InSb.

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Table 1. Comparison of present calculation (pseud.) of spin-orbit splittings and linear terms to experiment and LMTO calculations of Ref. 6. Units are eV and meVÅ for the splitting and linear terms, respectively.

	GaAs			InSb		
	Pseud.	LMTO	Exp.	Pseud.	LMTO	Exp.
s-o splitting	0.345	0.351	0.341[a] 0.350[b]	0.758	0.799	0.81 (1.5K)[c] 0.813 (4K)[d]
linear term	-3.42	-3.4,-3.6	——	-9.85	-9.2	|9.3|[e]

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d) R.L. Aggarwal, in Semiconductors and Semimetals, Vol. 9, eds. R.K. Willardson and A.C. Beer, (Academic, 1972) p 151.
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Table 2. Quadratic (C^2) and cubic (C^3) coefficients for the Γ_8 bands. The units are eVÅ^2 and eVÅ^3 for the C^2 and C^3 coefficients, respectively.

	GaAs	InSb
$C^2_{\Delta ab} = C^2_{\Delta cd}$	-6.9×10^1	2.2×10^1
$C^2_{\Lambda a} = C^2_{\Lambda d}$	-4.8	-5.6
$C^2_{\Lambda bc}$	-1.33×10^2	5.5×10^1
$C^2_{\Sigma a} = C^2_{\Sigma d}$	-1.32×10^1	-1.6
$C^2_{\Sigma b} = C^2_{\Sigma c}$	-1.24×10^2	5.1×10^1
$C^3_{\Delta ab} = C^3_{\Delta cd}$	-4.7×10^5	-8.0×10^4
$C^3_{\Lambda a} = C^3_{\Lambda d}$	absolute value $< 10^{-1}$	-1.5×10^3
$C^3_{\Lambda bc}$	0.00	0.00
$C^3_{\Sigma a} = C^3_{\Sigma d}$	-2.4×10^5	-3.6×10^4
$C^3_{\Sigma b} = C^3_{\Sigma c}$	2.6×10^5	3.7×10^4

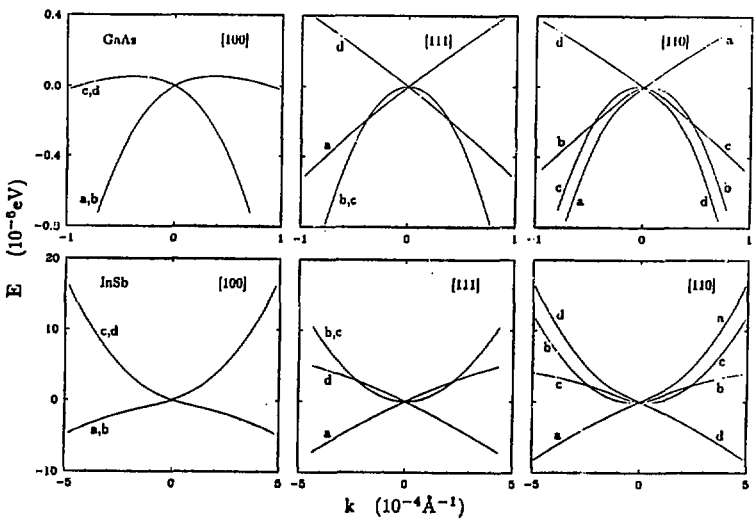

Figure 1. Band structures at the top of the Γ_8 valence bands for GaAs and InSb in the [100], [111], and [110] symmetry directions.