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Empirical formula for the spin-orbit splitting in semiconductors

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The spin-orbit splittings in elemental and compound semiconductors are shown to be linearly related with the atomic ionization potential. The relation is used to judge the acceptability of the different reported values of the splitting for various semiconductors. © 1995 American Institute of Physics.

Semiconductors are the basic materials for most of the current electronic and optoelectronic devices and their various physical constants are required to be known for the design of these devices. Spin-orbit splitting, Δ , is one constant, which is used to estimate the values of various other physical constants, e.g., the effective mass of electrons and holes,¹ the nonparabolicity parameter,² modified Luttinger parameters,³ and the interband matrix element.⁴ The value of the constant is also used in the analysis of photoluminescence⁵ and light absorption⁶ and in the design of lasers.⁷

Values of Δ have not, however, been obtained experimentally for all the semiconductors. Furthermore, even the values obtained in different experiments vary by large factors for some materials.⁸⁻¹⁰ It is, therefore, important to have a method for checking the estimated values and for choosing one among the many reported values. A method of checking may be obtained if the spin-orbit splitting is found to be related by a simple relation with an accurately known atomic property. It has been shown that the inverse of the dielectric constant,¹¹ and the melting point¹² vary linearly with the mean atomic number. On the other hand, the lattice constant and the zone-center optic phonon frequency¹³ have been found to be linearly related with the mean atomic ionization potential.¹⁴ Spin-orbit splitting being determined by the fields near the atoms like these constants is also likely to be correlated with the atomic ionization potential. The purpose of this communication is to explore this possible correlation.

Values of Δ , collected from different sources, are listed in Table I. It is seen that only estimated values are available for AlP, AlAs, CdSe, HgS, and HgSe and the reported values for GaP, InP, and AlSb differ, respectively, by factors of 1.6, 1.9, and 1.1. It may also be noted that compounds with a common anion have nearly equal values of Δ . Attempts were made earlier to obtain spin-orbit splitting of the compounds by combining suitably weighted atomic values.¹⁵ The required weighting for anions was found to be (2/3) for the III-V compounds and (3/4) for the II-VI compounds.¹⁶ We may conclude that the values of Δ for the compounds are determined mostly by their values for the anions. We have therefore, examined, possible correlation between Δ and the ionization potential, V_{ion} , for the group -IV, V, and VI atoms, listed in Table II.

The spin-orbit splitting, Δ , is plotted in Fig. 1 against V_{ion} for the group IV elements and for the anions of the compounds. It is seen that Δ generally decreases with increase in V_{ion} , but its value is not the same for the same value of V_{ion} . A general empirical relation cannot, therefore, be found between Δ and V_{ion} . However, when we consider

Δ 's and V_{ion} 's for group IV elements and II-VI compounds with a common group II element (for each of which only one value of Δ is reported), we find that Δ may be expressed by the following linear relation in terms of V_{ion} ,

$$\Delta = a - bV_{\text{ion}}, \quad (1)$$

with root-mean-square percentage errors (RMSPE) of 1.35%–3.5%. Values of a and b for the minimum value of RMSPE are given in Table III. For materials with different reported values of Δ , a linear relation, as found for elemental and II-VI semiconductors, was assumed to apply and a best fit was determined by so combining the values as to obtain a straight line with the least value of RMSPE. Values of a and b and the errors for the best fit are also quoted in Table III, for these materials.

The decrease of Δ with increase in V_{ion} , as observed from the data, may be understood from the following considerations. The ionization potential, V_{ion} is determined by the field in the outer region of the atoms and its value should decrease with decrease in this field. As the atomic number Z increases within a group, the outer shells are filled and the potentials spread more and more causing a decrease of field

TABLE I. Spin-orbit splitting, Δ , in semiconductors (in eV).

Material	Δ^a	Δ^b	Δ^c	Δ^d
Si	0.04	0.044	0.044	0.044
Ge	0.29	0.29	0.29	0.28
α -Sn	0.77	0.8	0.8	0.81
AlP	0.05 ^e	0.06 ^e	-	0.06
GaP	0.08	0.127	0.08	0.08
InP	0.13	0.21	0.108	0.108
AlAs	0.28	0.29 ^e	0.3	0.29
GaAs	0.34	0.34	0.341	0.34
InAs	0.38	0.38	0.38	0.38
AlSb	0.75	0.75	0.673	0.68
GaSb	0.77	0.8	0.76	0.78
InSb	0.81	0.82	0.85	0.85
ZnS	0.07	0.07	-	0.07
CdS	0.07	0.066	-	0.07
HgS	0.07 ^e	0.13 ^e	-	0.07
ZnSe	0.43	0.43	-	0.45
CdSe	0.42 ^e	0.42 ^e	-	0.45
HgSe	0.45 ^e	0.48 ^e	-	0.47
ZnTe	0.92	0.93	-	0.91
CdTe	0.91	0.92	-	0.91
HgTe	1.00	0.98	-	0.96

^aRef. 8.

^bRef. 9.

^cRef. 10.

^dValues computed from the empirical relations.

^eEstimated values.

TABLE II. Ionization potential, V_{ion} , of atoms^a (in eV).

Atom	V_{ion}	Atom	V_{ion}	Atom	V_{ion}
Si	8.151	P	10.485	S	10.360
Ge	7.898	As	9.814	Se	9.751
α -Sn	7.344	Sb	8.640	Te	9.010

^aRef. 13.

in this region. V_{ion} , therefore, decreases in a group as Z increases, i.e., in the order Si, Ge, Sn for group IV. P, As, Sb for group V and S, Se, Te for group VI elements. On the other hand, values of Δ are determined by the fields associated with the core states¹⁷ and as this field increases with Z , Δ also increases. We may, therefore, conclude that Δ should increase as V_{ion} decreases with increase in Z . However, although the general nature of variation of Δ with V_{ion} may thus be explained, the physics of the linear relation is difficult to explain and the relation should be considered to be empirical. We may, however, conclude from the close fit of

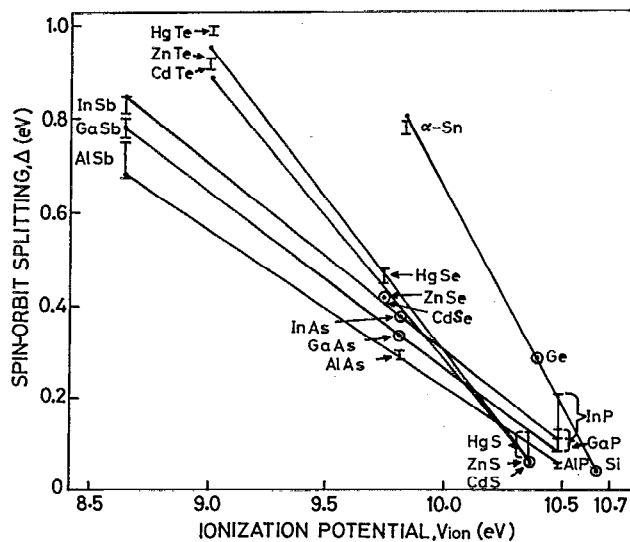


FIG. 1. Spin-orbit splitting vs the ionization potential, V_{ion} , abscissa gives for the III-V compounds and II-VI compounds, V_{ion} of the anion, and for the elemental semiconductors $V_{ion}+2.5$. Extreme reported values are shown by bars.

TABLE III. Constants a and b and the root mean square percentage error (RMSPE) for the empirical relations.

Semiconductor	a	b	RMSPE
Elemental	7.817	0.9536	1.35
Aluminum compounds	3.590	0.337	1.1
Gallium compounds	4.057	0.379	1.2
Indium compounds	4.337	0.403	0.25
Zinc and selenium compounds	6.340	0.605	2.7
Mercury compounds	6.871	0.657	3.6

the data with the empirical straight lines that the estimated values for AlP, AlAs, HgS, and HgSe are also the likely values. Furthermore, for the three compounds, GaP, InP, and AlSb, for which widely different values are reported, the smaller of the extreme values are the most likely.

In conclusion, the spin-orbit splitting in elemental, and compound semiconductors with a common group III and a common group II element are found to be linearly related, respectively, with the ionization potential of the group IV, group V, and group VI atoms. These relations may be used to check the acceptability of a particular reported value for a semiconductor.

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