

ble contributions to the sum in (1), interband and excitonic, with  $\omega_j - \omega_{j'} = \omega_g$  in both cases, and with oscillator strengths  $f_1$  and  $f_2$ , respectively, given by

$$f_1 = \omega_g(\text{Ge})/\omega_g, \quad (4)$$

$$f_2 = 1 - f_1. \quad (5)$$

Harrison's model retains only  $f_1$ , whereas our model includes  $f_1 + f_2$ . From an inductive viewpoint the cancelation of the two effects, as required by the sum rule, is a great simplification. It is just this cancelation which makes possible a chemical theory, i.e., one which explicitly exhibits effects dependent on size and on the valences  $N$  and  $8 - N$  or the valence difference  $8 - N - N = 2(4 - N)$ .

At present there are no complete deductive treatments in semiconductors of excitonic effects (sometimes called local-field corrections) which would explain the observed cancelation. There have been several efforts on the subject recently,<sup>9</sup> but none of them has attempted to establish broad chemical trends of the kind required to differentiate between Harrison's and our own models. Because our model incorporates the sum rule (2) in the simplest possible manner, and because it is both classical and chemical (in the previous sense) I believe it is the one to be preferred in most cases.

In view of the above, I recommend caution in considering the use of Harrison's model. There has been solid work extending and refining our ideas, e.g., the derivation of orbitally dependent electronegativities,<sup>10</sup> which resolves the discrepancies between Pauling's table of electronegativities and our table, as well as work on ionic

contributions to structural energies in intermetallic compounds.<sup>11</sup> Because of this excellent work the entire field of theories of electronegativity will soon be ripe for review again.

<sup>1</sup>J. C. Phillips, Rev. Mod. Phys. **42**, 317 (1970).

<sup>2</sup>J. C. Phillips, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1966), Vol. 18, p. 56; D. L. Greenaway and G. Harbeke, *Optical Properties and Band Structure of Semiconductors* (Pergamon, New York, 1968); M. Cardona, in *Solid State Physics*, Suppl. No. 11, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1969); M. L. Cohen and V. Heine, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1970), Vol. 24; J. C. Phillips, *Bonds and Bands in Semiconductors* (Academic, New York, 1974).

<sup>3</sup>J. C. Phillips, Phys. Rev. Lett. **20**, 550 (1968).

<sup>4</sup>L. Pauling, *The Nature of the Chemical Bond* (Cornell Univ. Press, Ithaca, N. Y., 1960).

<sup>5</sup>W. A. Harrison, Phys. Rev. B **8**, 4487 (1973).

<sup>6</sup>W. A. Harrison and J. Ch. Phillips, Phys. Rev. Lett. **33**, 410 (1974); but see J. A. Van Vechten, Phys. Rev. B (to be published), for a deeper theory.

<sup>7</sup>K. C. Pandey and J. C. Phillips, Phys. Rev. Lett. **32**, 1433 (1974).

<sup>8</sup>J. A. Van Vechten, Phys. Rev. **182**, 891 (1969).

<sup>9</sup>S. G. Louie, J. R. Chelikowsky, and M. L. Cohen, Phys. Rev. Lett. **34**, 155 (1975), find that local-field effects shift oscillator strength to higher energies. J. A. Van Vechten and R. M. Martin, Phys. Rev. Lett. **28**, 446, 646(E) (1972), and W. R. Hanke and L. J. Sham, Phys. Rev. Lett. **33**, 582 (1974), find that excitonic effects shift oscillator strength to lower energies, in qualitative accord with the contribution we have schematically represented by  $f_2$ .

<sup>10</sup>J. St. John and A. Bloch, Phys. Rev. Lett. **33**, 1095 (1974).

<sup>11</sup>E. S. Machlin, Acta Met. **22**, 95, 109, 367 (1974).

## Reply to Phillips's Comment on the Bond-Orbital Model

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The central question of Phillips's Comment, that concerning the dependence of dielectric constant on band gap in polar semiconductors, is extracted and answered theoretically and in terms of experiments. My conclusion differs from his.

I agree that the variation of oscillator strengths in isoelectronic series of increasing polarity, such as Ge, GaAs, ZnSe, CuBr, is very important. This is particularly true for Phillips's ion-

icity theory<sup>1</sup> since the cornerstone of the work is the assumption that the dimensionless oscillator strength can be taken as constant in going from Eq. (1) to Eq. (3) in Phillips's Comment<sup>2</sup>; that

step is basic to the definition of ionicity in terms of the dielectric constant and the entire structure rests on it. In contrast, the dielectric constant derived in the bond-orbital model<sup>3</sup> shows an additional dependence upon polarity due to the spatial separation of the bonding and antibonding states. This yields a dependence of  $\epsilon_1 - 1$  upon the band gap of the form  $(\hbar\omega_g)^{-3}$  in an isoelectronic series, or a proportionality of the dimensionless oscillator strength to  $\hbar\omega_g^{-1}$ . Note that bond length does not vary appreciably in such a series.) It is desirable to state the problem clearly and to seek a test of these significantly different results. We should not selectively bury the results we do not like by introducing new parameters to absorb the discrepancy.

The oscillator strength for a particular transition can be written in terms of the matrix elements of the coordinate between those states<sup>4</sup> or, with use of a familiar identity,<sup>5</sup> in terms of the matrix elements of the gradient. The latter form is

$$f_{ij} = 2\hbar^2 |\langle i | \nabla | j \rangle|^2 / m\hbar\omega_{ij}.$$

The assumption upon which Phillips has based his theory, then, is that the square of the matrix element,  $\langle i | \nabla | j \rangle^2$ , is proportional to the band gap,  $\hbar\omega_g = \hbar\omega_{ij}$  for the two-level model. The bond-orbital model predicts it to be independent of the gap. The square of the matrix element has long been known experimentally to be independent of polarity, or ionicity, in an isoelectronic series,<sup>6</sup>

in support of the bond-orbital model but contrary to Phillips's assumption. The recent calculations by Chelikowsky and Cohen, shown in Phillips's Table I,<sup>2</sup> independently support this conclusion as have earlier calculations. This simply means that some of the oscillator strength is transferred to higher energies. There seems not to be theoretical nor experimental support for the assumption upon which the ionicity theory is based. It may have seemed plausible at the outset and there may not have been motivation to test it subsequently. It appears now that the assumption was incorrect and I do not find the current effort to rescue it convincing.

<sup>1</sup>J. C. Phillips, Rev. Mod. Phys. **42**, 317 (1970).

<sup>2</sup>J. C. Phillips, preceding Comment (Phys. Rev. Lett. **34**, 1196(C) (1975)).

<sup>3</sup>W. A. Harrison, Phys. Rev. B **8**, 4487 (1973); W. A. Harrison and S. Ciraci, Phys. Rev. B **10**, 1516 (1974). Note that in the latter the defining standard for the gap was taken to be the absorption peak  $E_2$ , not the dielectric constant.

<sup>4</sup>See, for example, J. M. Ziman, *Principles of the Theory of Solids* (Cambridge Univ. Press, Cambridge, England 1964), p. 225.

<sup>5</sup>L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), 3rd ed., p. 404.

<sup>6</sup>P. Lawaetz, Phys. Rev. B **4**, 3460 (1971); see in particular the concluding paragraph. Noted also by J. C. Phillips, *Bands and Bands in Semiconductors* (Academic, New York, 1973), p. 121.

## Is a "New Scaling Hypothesis in High Energy Collisions" Needed?

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The experimental results used by Dao *et al.* to support a "scaling-in-the-mean" hypothesis for semi-inclusive processes can also be reproduced by a simple *Ansatz* for the invariant cross section obeying Feynman scaling, Koba-Nielsen-Olesen multiplicity scaling, and factorization in longitudinal and transverse momenta.

In a recent Letter, Dao *et al.*<sup>1</sup> observed a striking regularity in semi-inclusive production of  $\pi^-$  in  $pp$  collisions. They studied the production cross section as a function of the prong number  $n$ , the pion longitudinal momentum  $p_L$ , and its transverse momentum  $p_T$ . With  $\langle p_L \rangle_n$  denoting the mean value of the longitudinal momentum for a given prong number, they find that the differen-

tial cross section<sup>2</sup>  $(\langle p_L \rangle_n / n\sigma_n) d\sigma_n / dp_L$  is a function only of the ratio  $p_L / \langle p_L \rangle_n$  and is independent of both  $n$  and the total energy  $s$ ; this may be called "scaling-in-the-mean" for the longitudinal cross section. An analogous observation was made for the transverse-momentum distribution. Dao *et al.* use this observation to propose scaling-in-the-mean as a general property for semi-