Proceedings, 6th Int'l Tin

combination of two types of phenomena. Much

metal-

electron-

nonmetal transition

interactions

methods show the band energies to be nonlinear functions of the potential parameters.

We may express this as $E_{AC} = pV_{AC} + q\zeta^2_{AC} + \ldots$, where p and q are coefficients and

integrals

was able to produce almost any desired value of b, simply

by making small adjustments

band parameters without

spoiling thereby the quality

ZnSe. To [illegible] they find $b_x = -0.01$ eV [illegible] and others

[illegible]

dominant. I find this conclusion to be untenable for all isovalent semiconductor

[illegible]

C = P, As, Sb), have shown that their band gaps are substantially smaller than those of their binary analogs (e.g., ZnSe is the bi[illegible]

[illegible]

reduction of band gaps in response to the internal stress exerted by the unequal bond lengths is common to real chalcopyrites (e.g., $CuInSe_2$) and to pseudo chalcopyrites

[illegible]

and 1-3 eV for the III-III-V pseudo chalcopyrites. One can express [illegible] contribution to the [illegible]

[illegible]

difference between A and B. But even for [illegible], ΔE^s can differ from zero [illegible] $\neq 1/4$, hence we have the [illegible] second order term [illegible] that depends on the "average" of A and B. To evaluate ΔE^s we need to know the equilibrium [illegible]

[illegible] values. The results agree [illegible]

[illegible] In addition to this structural contribution [illegible] we find a chemical [illegible] ΔE^{chem}. It results from the fact that even if $u = 1/4$, (i.e., when [illegible]) the electronic charge density can distribute itself differently [illegible] the A-C [illegible]

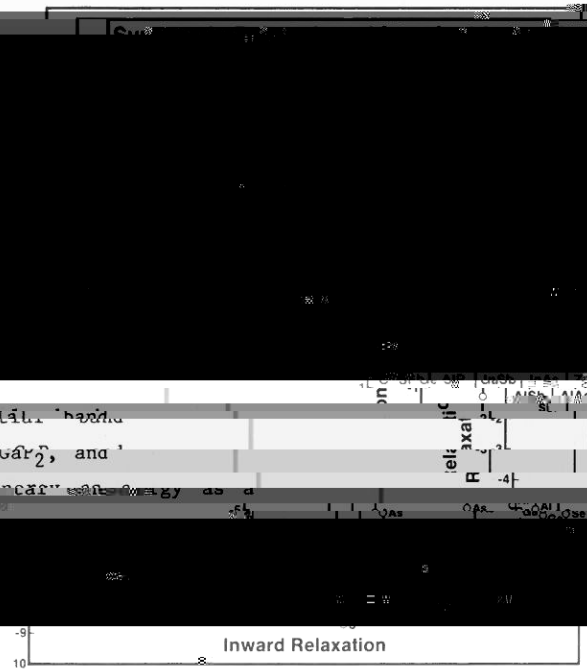

Fig. 1: Calculated bond relaxation (open circles) for isovalent impurities in semiconductors (abscisa). Astriks denote experimental EXAFS values.