CHEMICAL TRENDS AND UNIVERSALITIES IN THE SPECTRA OF

TRANSITION METAL IMPURITIES IN SEMICONDUCTORS

[redacted]

fixed configuration (say, $e^m t_2^n$) contains the average energy $\hat{E}_{m,n}(A,B,C)$ of all single-configuration energies that evolve from (m,n). Here, A is the totally symmetric interelectronic repulsion, and B,C are the anisotropic multiplet Racah parameters. The true [illegible]

[illegible]

incorporate explicitly the separation of average MF effects from multiplet corrections.

This general formalism can be applied in two ways. First, one could compute from MF wavefunctions all of the symmetry and spin-dependent anisotropic many-electron integrals underlying $\Delta E^{(1)}_{m,n;m',n'}(B,C)$, as well as the MF energy separations $\Delta_{eff}(m,n;m',n')$, and insert them into the general matrix equations (1) to obtain the multiplet spectra and their MF vs MC components. Alternatively, one may wish to establish the magnitude and trends in the multiplet corrections [illegible] experimental data itself, using the integrals of the theory as potential parameters. In view of the number of independent integrals [illegible] of the scatter [illegible] characterizing all occupied impurity-induced e and t_2 orbitals by the orbital deformation parameters λ_e and λ_t, as in Ref. (4), different from those in Ref. (3), measuring the ratio of the interelectronic interactions [illegible]

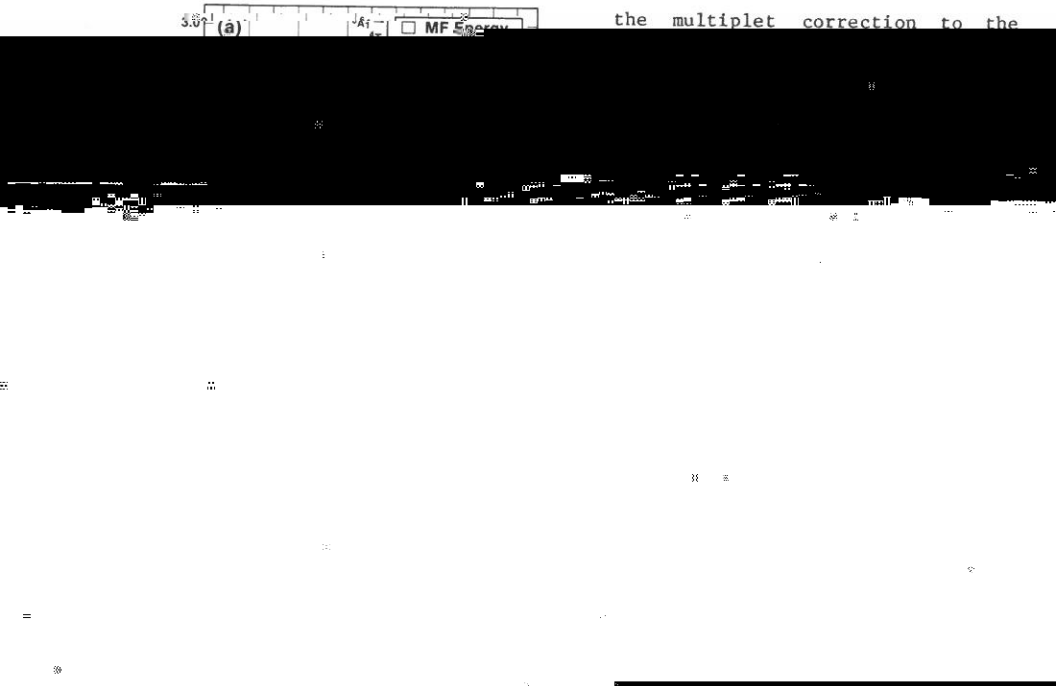
[illegible]

[illegible] of the 3+ and 2+ ions is the MC for donor [illegible] in MC's for the ground state [illegible] the acceptor transition energies [illegible] transition energies in III-V's and [illegible] we hence have a separation

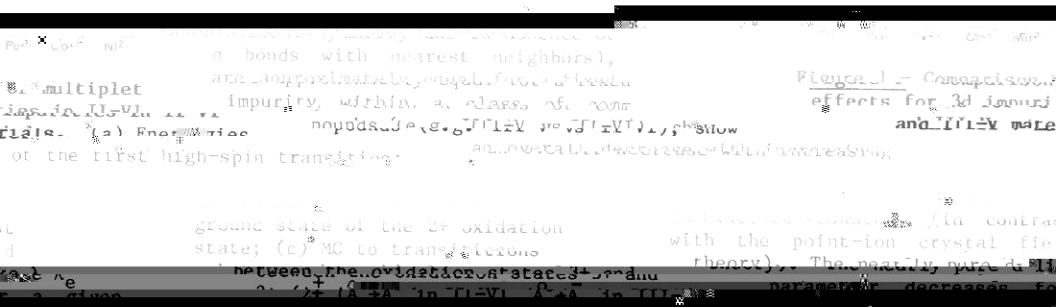
$$E_D(0/+) = \Delta E^{N,N-1}_{MF} + \Delta E^{N,N-1}_{MC}, \quad (1)$$

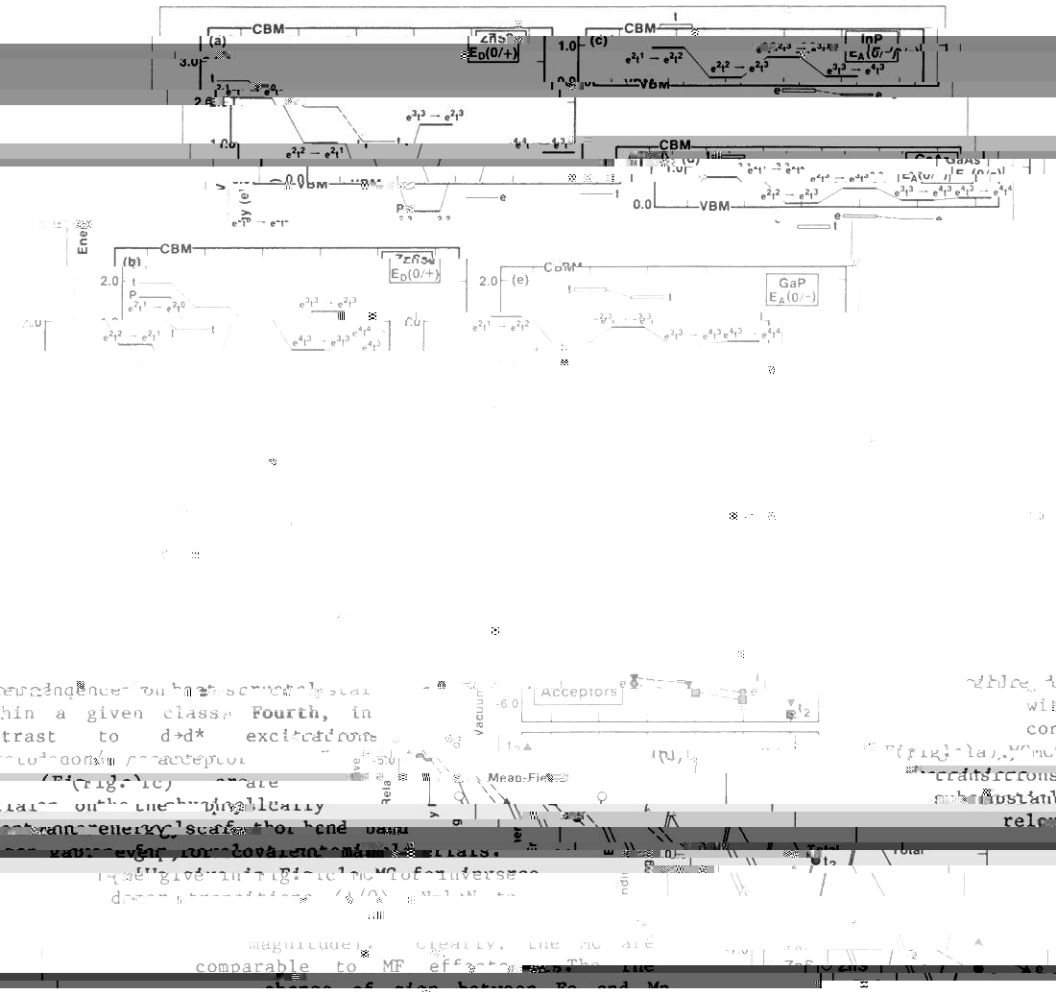
$$E_A(-/0) = \Delta E^{N,N+1}_{MF} + \Delta E^{N,N+1}_{MC}$$

[illegible] N electrons. Fig. 2 displays the [illegible] for acceptors and the negative for the [illegible] where the neutral system A^0 [illegible] electron correction ΔE [illegible] for donors. Finally, $\Delta E^{N,N+1}_{MC} - \Delta E^{N,N-1}_{MC}$ [illegible] correction $\Delta E^{N,N-1}$ [illegible]



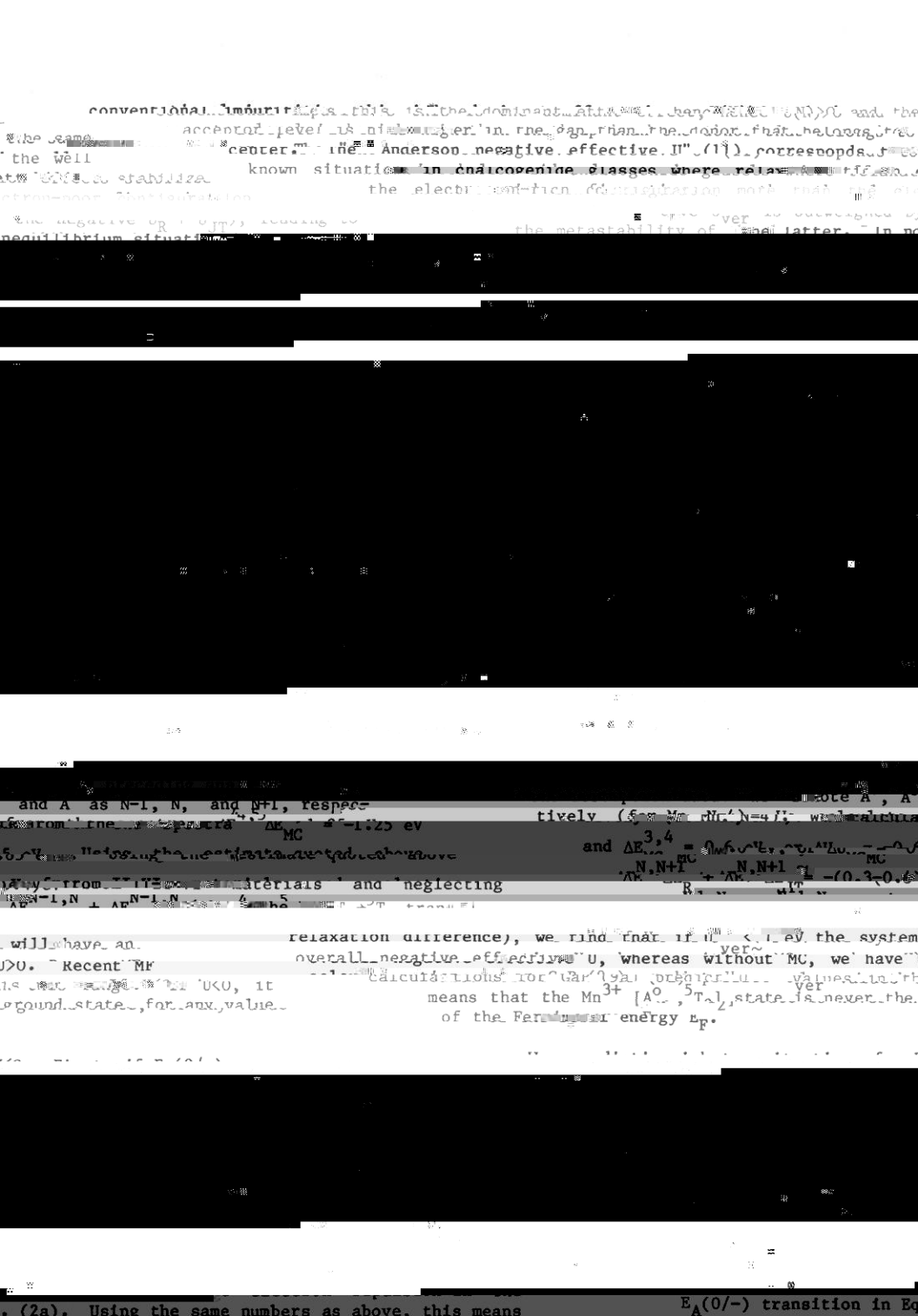
the multiplet correction to the




(a)
CBM
ZnS
$E_D(0/+)$
3.0
2.0
1.0
0.0
VBM
(b)
CBM
ZnSe
$E_D(0/+)$
2.0
1.0
0.0
VBM
(c)
CBM
InP
$E_A(0/-)$
1.0
0.0
VBM
(d)
CBM
GaAs
$E_A(0/-)$
1.0
0.0
VBM
(e)
CBM
GaP
$E_A(0/-)$
2.0
1.0
0.0
VBM
Ene
P
e

Acceptors
Vacuum
-6.0
Mean-Fie
Rela
Total

[redacted]



. (2a). Using the same numbers as above, this means

$E_A(0/-)$ transition in Eq

that $\Delta E^{4,3}_{ver} \lesssim 1.6$ eV. Recent MF calculations (9a) show that this is close to, but not the case for GaP:Mn, but could be the case for

bonds cannot provide enough energy to transform the atom entering the crystal (d^5 Mn) into the neutral state (d^4) and lower energies are attained by the d^5 configuration (A. Zunger, The observed (positive) acceptor

(9) (a) A. Singh and A. Zunger (to be published);
Solid State Comm.
J. Phys.