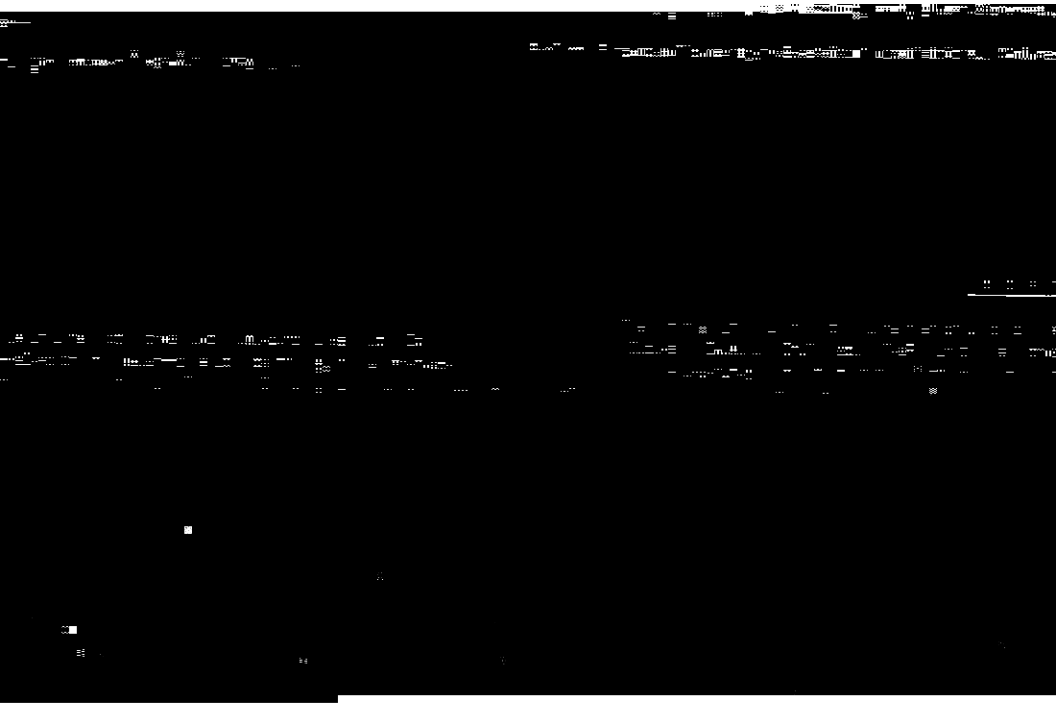
CHEMICAL TRENDS AND UNIVERSALITIES IN THE SPECTRA OF

TRANSITION METAL IMPURITIES IN SEMICONDUCTORS



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 Racah parameters. The true ... multiplet ...

... 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 ... experimental data itself, using the integrals of the theory as fitting parameters. In view of ... the number of independent integrals ... of the scarcity of data ... occupied impurity-induced e and t_2 orbitals by the ... characterizing a ... deformation parameters λ_e and λ_t [as in Ref. (4)], different from those in Ref. (3)], measuring the ratio of the interelectronic interactions to those in the free ion [characterized by ...

... of the 3+ and 2+ ions is the MC for donor ... in MC's for the ground states ... the acceptor transition energies ... in III-V's and II-VI's we hence have a separation

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

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

where the neutral system A^0 has N electrons. Fig. 2 displays the many-electron correction ΔE ... for acceptors and the negative ... for the ... for donors. Finally, ... ΔE_{MC} ... correction ...

the multiplet correction to the

...

σ bonds with nearest neighbors), are approximately equal for a fixed impurity, within a class of compounds (e.g. II-VI or III-V), show an overall decrease with increasing

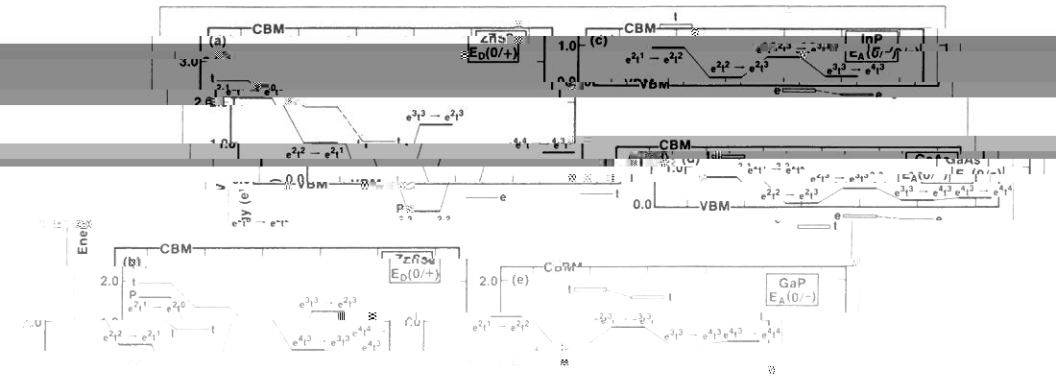
... (in contrast with the point-ion crystal field theory). The nearly pure d ... parameter decreases for

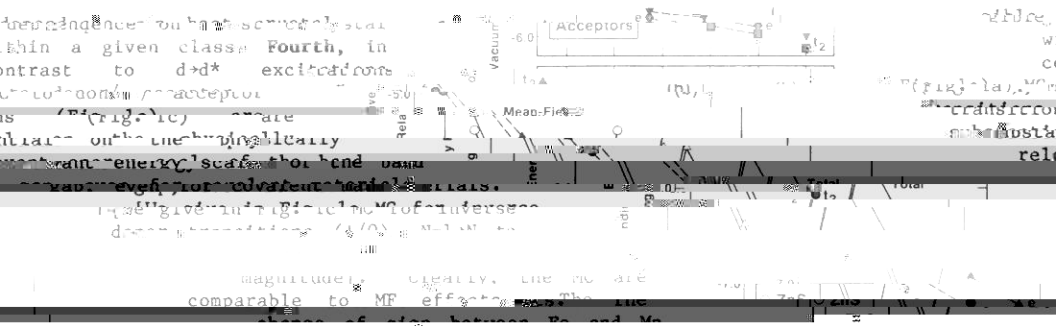
... multiplet ... ies in II-VI ... als. (a) Energies of the first high-spin transition ... ground state of the 2+ oxidation state; (c) MC to transitions between the oxidation states 3+ and 2+ ...

Figure 1 – Comparison ... effects for 3d impurit... and III-V mater...

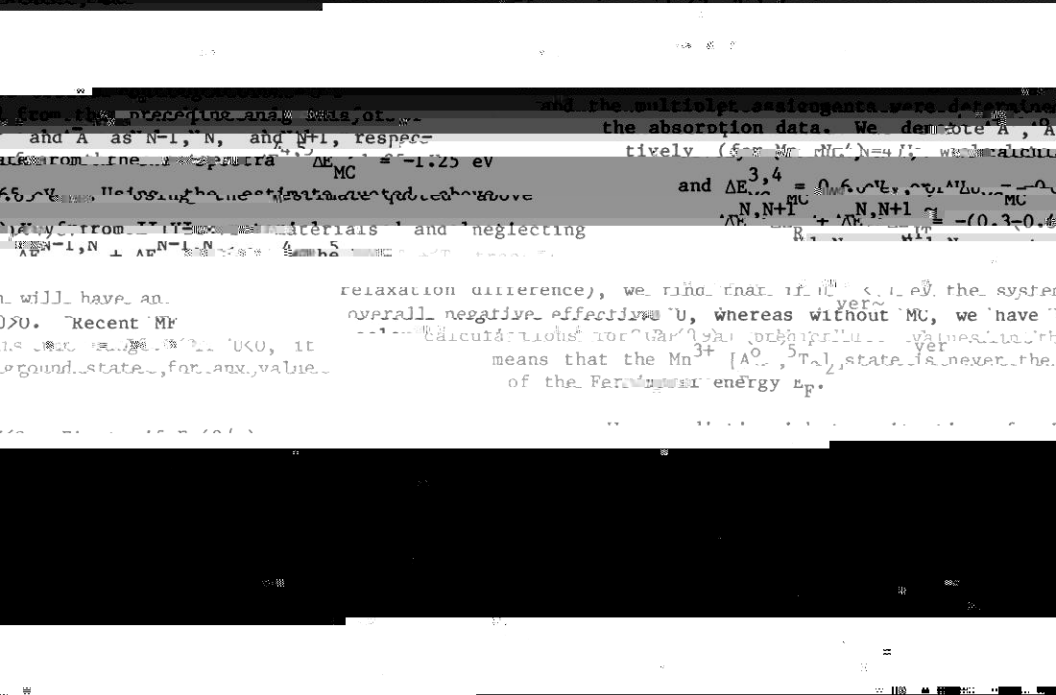
...

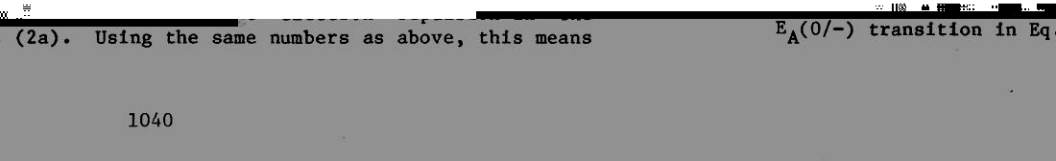
impurity to the other (e.g. the correction reduces the excitation energy for Fe but ...


(a)
CBM
ZnS
$E_D(0/+)$
3.0
2.6
1.0
0.0
VBM
(c)
CBM
InP
$E_A(0/-)$
1.0
0.0
VBM
CBM
GaAs
0.0
VBM
(b)
CBM
ZnSe
$E_D(0/+)$
2.0
(e)
CBM
GaP
$E_A(0/-)$
2.0


Acceptors
Vacuum
-6.0
Mean-Field
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 MR calculations (9a) show that this is not the case for GaP:Mn, but could be the case for to, but

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^6 configuration (A^0 hole). The observed (positive) acceptor

(9a) A. Singh and A. Zunger (to be published);