AND ALEX ZUNGER
Solar Energy Research Institute, Gol
den, CO 80401.

ABSTRACT

Self-consistent spin-unrestri
icted all-electron Green's function calcula-
tions are reported for
the first time for a series of interstitial 3d
impurities
in silicon. The calculations performed within the local
central hyperfine coupling constants, (iii) chemical trends in donor and

have been postulated that: (i) The level ordering for all 3d

consequence of
hybridization. (iv)
transitions [4] were interpreted

a dynamic Jahn-Teller effect [5], not due to covalent
Subsequent measurements for donor and acceptor

impurities in wider

on contribution to various excitation
one-electron theory [10], it was possible
electron part of the excitation energies, and

proportion of one electron vs many electron
processes. Using the self-consistent
to compute the mean field one-electron

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[illegible]

and Co. Figure 2 shows the calculated and observed [1] spin st

[illegible]

values from $g = g_S + g_L$ [illegible] where [illegible] are the electron spin and orbital angular momentum con[illegible]

[illegible]

the impurity orbital at the Fermi energy. In the case of $J=L-1$, $S=3/2$, 2 and

J=1/2. A is given by A = $2\mu_B g_J \beta \langle r^{-3}\rangle[g_J - \frac{k}{} g]$, where $g_J \approx$ 2.0023

[illegible]	5/2	5/2	2.0023	0.	−0.0007	1.9986	1.9978	+11.0	+10.67	
$^{53}Cr^0$	2	1	1	2.0035	0.0878	−0.0085	3.0828	2.97	+14.0*	+15.9
[illegible]	2	1	1	2.0035	0.0887	−0.0147	3.1064	3.311	[illegible]	

[illegible]

...ptors in Si:Sd. Our results follow the experimental ... the first donor and acce... trends [4], although...

...ugh they ... were [illegible] ed to ... Franck-Condon ...

... transitions (and in principle, should ... be ... optical excitation

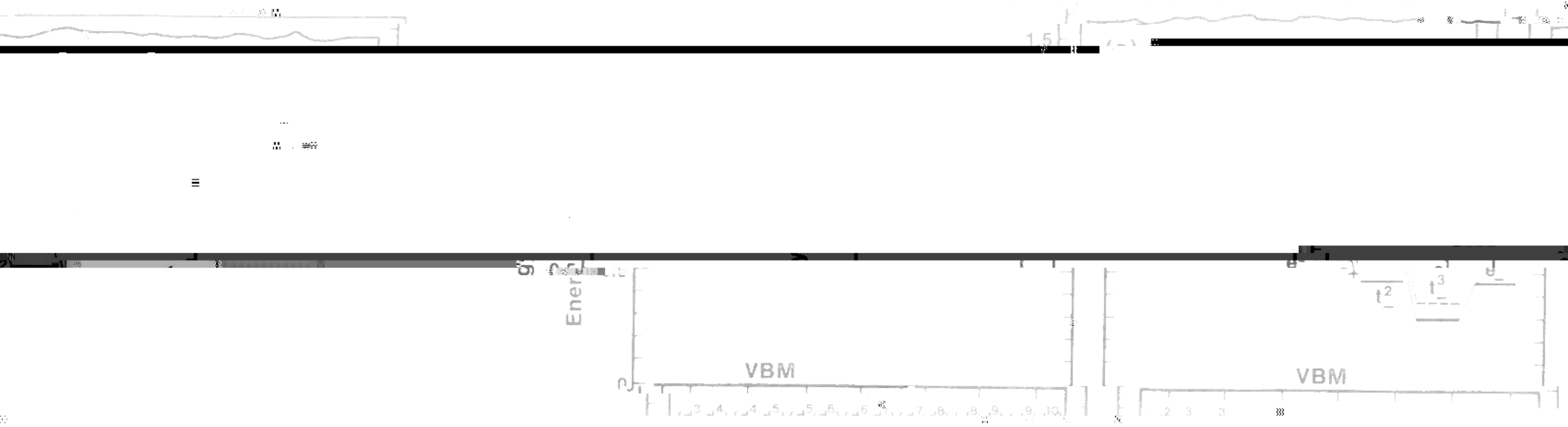
[illegible]

... elements [illegible]

simply suggests that within the impurity subspace there is no exact cancellation of spin-up and spin-down densities. This corresponds to a single-site-like free spin density wave.

...s of effective ... nifested by the fact

5. The exchange-correlation ... negative ... the positiveness ... interelectronic Coulomb repulsions for impurities is ma...



than acceptor transitions if both commence from the same orbital. In general, their separation U can be thought of as

tion (e.g. $t_2^3e^1 \rightarrow t_2^2e^2$ and $t_2^2e^1 \rightarrow t_2^1e^2$) can ... exchange energy ... excita ... We find in our calculation that this is the case ... the Coulomb repulsi

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