HYPERFINE INTERACTION OF THE IRON IMPURITY NUCLEI AT THE TETRAHEDRAL INTERSTITIAL SITE IN SILICON

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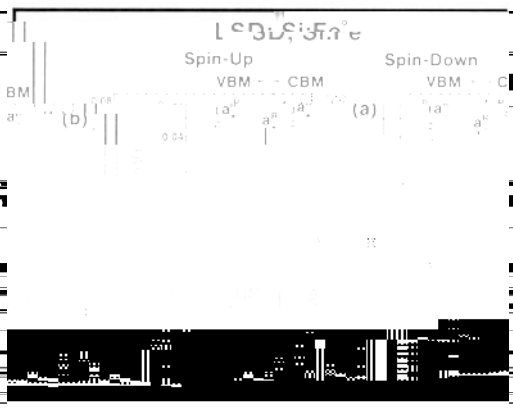
Most electronic structure calculations on transition metal impurities in semiconductor[1-6] were performed within the local density formalism[7], implemented either in an extended-crystal Green's function approach[1-2], or within finite cluster models[3-6]. Involving a local (statistical) approximation to exchange and correlation, the local density approximation, much like its predecessor, the Thomas-Fermi model involves an unphysical interaction of each spin-orbital with itself[8] (self-interaction). Whereas

significant effect on localized states. Such is the case for isolated transition atoms, where a self-interaction corrected model shows[8] that relative to LSD (i) the 3d orbitals move to substantially more negative energies (increasing thereby the s-d separation), (ii) the 3d orbitals become more localized, whereas the non-d (valence)

in the self-consistent potential, we economize on the basis size using only the ls-



the LSD formalism, and Fig. 1 (right) gives the corresponding results obtained in the LSD-SIC calculation. The major effects of SIC are seen to be: (i) a shift of all occupied pure d levels (i.e. e-representation) to more negative energies (e.g. e_+^b by 0.42 eV, and e_+^a by 0.33 eV), as they are relieved from the (repulsive) self-interaction, (ii) a corresponding upward shift of the occupied orbitals that contain substantial non-d character (e.g. the t_+^b, t_-^b and t_-^a move up by 0.09 eV, 0.4 eV and

Table I: Comparison of different orbital contributions (in KG) to the contact hyperfine field in $Si:Fe^{o}$.

Table II: Effective occupation numbers of Fe in $Si:Fe^{o}$.

Note that whereas the LSD formalism emphasizes the difference between spin-up and

occupied and unoccupied orbitals. Hence whereas the $e^a - e^a$ exchange splitting be-

is three times larger in LSD-SIC predominantly due to an upwards shift in e^a. This

upward shift of e^a has an important physical consequence. Whereas in the cluster and