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

H. Katayama-Yoshida and Alex Zunger Solar Energy Research Institute, Golden, Colorado 80401, USA

Most electronic structure calculations on transition metal impurities in semiconductor¹⁻⁶ were performed within the local density formalism⁷, implemented either in an extended-crystal Green's function approach¹⁻², or within finite cluster models³⁻⁶. 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 itself⁸ (self-interaction). Whereas

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	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)
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interaction, (ii) a corresponding <u>upward</u> 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

in the self-consistent potential, we economize on the basis size using only the 1s-

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Table I:	Comparison of different orbital Table II: Effective occupation
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