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Spin-Up
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=147.6—152.2 kG. We find a spin density at the
Fe nucleus of Sp(0) = —0.220 a.u. ', in reasonable
agreement with the observed values 4 of
esp(0) i =0.282-0.299 a.u.. The negative H„r
and Bp(0) result from the preferred expulsion of
spin-up density from the core region by the Coulomb repulsion between the core electrons and the unpaired 3d electrons. Third, we find for Si:Fe that the crystal-field splitting exceeds the exchange splitting (b /AqF=0. 88), and hence the

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ed only through massive lattice relaxations.
The resolution to the apparent dichotomy be-
tween the covalently delocalized and atomically lo-
calized models for Si:Fe lies therefore in this self-
regulating response and in the fact that different or-
bitals are responsible for the different aspects of the localization (duality): The contact spin density and hyperfine field are decided by the hyperlocalized core states, the magnetism is largely contributed by the localized valence-band resonances, and the donor
ionization, with its attendant high-spin configura-
tion, and the consistancy of the isomer shift are de-cided by a combination of delocalized gap states and the feedback (self-regulating) response of the valence-band resonances to excitations of the outer states.

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tE. R. Weber, Appl. Phys. A 30, 1 (1983(This