TRANSITION METAL IMPURITIES IN SEMICONDUCTORS

[illegible] to understand the [illegible]

[illegible] of 3d impurit[illegible] [illegible]

reviewed recently in Ref. 1), the electronic structure of 3d [illegible] impurities in semiconductors has received theoretical attention only rather recently.2 Rapid progress has, however, been made in this area, [illegible] techniques including [illegible] through [illegible] of [illegible] [illegible] cluster model[illegible], continued fraction, Extended Huckel methods[illegible]

[redacted]

individually[illegible] [illegible] [illegible]ities). This dichotomy [illegible] numerous text books and review articles and constitutes the working [illegible]

[illegible]

in semiconductors are "localized", note the following:


300
Free Atom
Manganese impurity

atomiclike high-spin (Hund's rule) ground states (Fig. 1), suggesting that as large as crystal field effects may be, exchange effects [illegible] (increasing with localization) usually outweigh them [illegible] existence of only small [illegible] energies suggest [illegible]

[illegible]

neighbors) suggests that the [illegible] wavefunctions may be [illegible] shell of [illegible]

[illegible] had convinced me that the only correct way to think about these systems is to describe them as **atomically localized and covalently delocalized at the same time** [illegible] duality [illegible] the classical vs. the quantal [illegible] light [illegible] I describe a few illustrations of this in the next section.

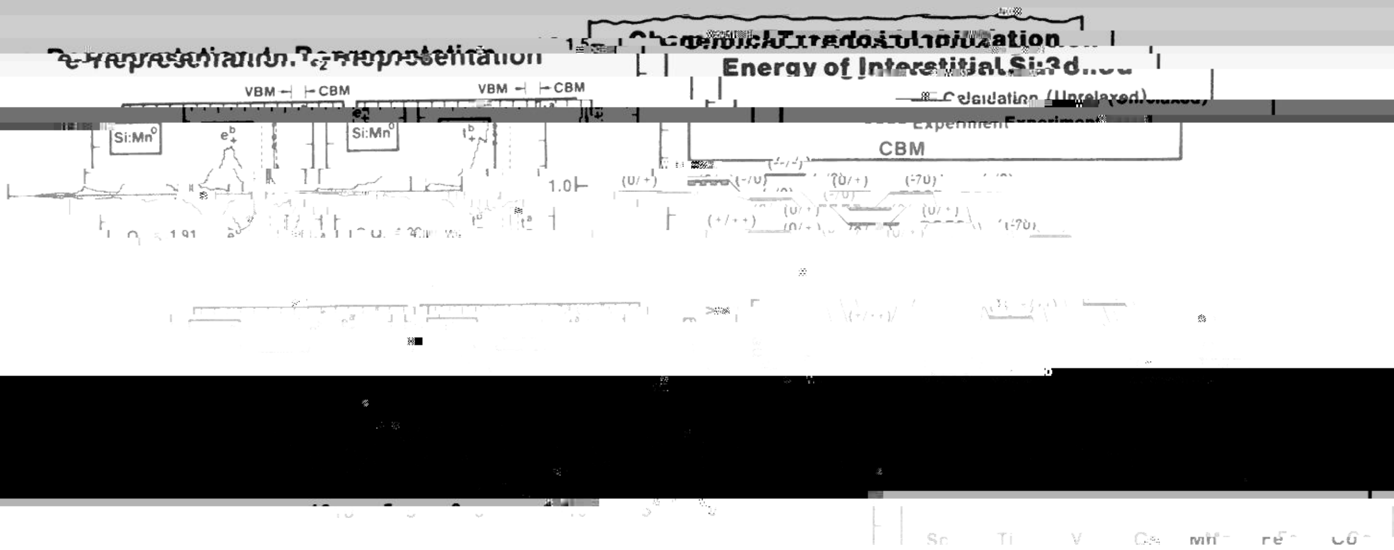
[illegible]

[illegible] naturally inside the [illegible] band ionic material, its d orbital energies fall [illegible]

[illegible] that (external) perturbations exerted on [illegible] most crystals, the sense [illegible] ionization [illegible] this ion (e.g. [illegible]

[illegible] valence bands, and only [illegible] ized resonances within the [illegible] shadow of its [illegible] band gap region. This is [illegible]

[illegible]



regulating response (analogous to homoestasis in biological systems), explains also why so many different

to note that only direct

delivery by this self-regulating

compensating contributions to the impurity

A. It's theorem, however

interactions are screened effecti

have hence

charge, both types of levels contribute in the same direction to the

This result predicts also that spin-densities (as observed

change with ionization

than that of the impurity.

The occurrence of hybridized valence band resonances is also largely responsible for the covalent

ergies

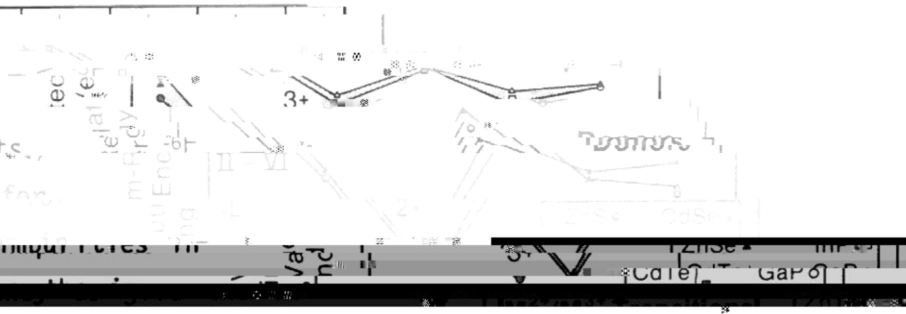
by atomic relaxation

direct calculations[7] of the force exerted by the impurity on its ligands has shown for interstitial impurities in Si that the first

shell containing 4 atoms moves outwards, whereas the second

of atomic-like Hund's rule ground states [illegible] the characteristic peak [illegible] of the [illegible] ioniza- [illegible]

[illegible] calculated [illegible] acceptor energies agree rather well with experiments (e.g., see Fig. 6 for interstitial impurities in Si), [illegible]



While the [illegible]

[illegible] the intrinsic valence band offset [illegible] the two semiconductors, thereby providing complementary information to that deduced by photoemission from interfaces [illegible] barriers [illegible]

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