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## First Principles Cluster Study of Electronic Structures, Locations and Hyperfine Interactions of Isolated Atoms and Ions in Silicon

### Summary

The electronic structures of very dilute transition metal (TM) atom and ion ( $Mn^0$ ,  $V^{2+}$ ,  $Cr^+$ , and  $Mn^{2+}$ ) complexes in silicon hosts have been studied using the Hartree-Fock procedure [1,2] combined with many-body perturbation theory with the aim to study the locations of TM atoms and ions and their hyperfine interactions. The clusters studied involved the TM atom and ions at the hexagonal interstitial (Hi), tetrahedral interstitial (Ti) and substitutional (S) locations, with the TM atoms and ions occupying a preexisting vacancy for the substitutional case. The nearest and next nearest neighbors of the TM atom and ions were included in the clusters for all of the sites studied. The energies of the centers were also studied for small variations in positions of the TM atom and ions along the  $\langle 111 \rangle$  axis, and perpendicular to this direction. From the results of these studies, it is concluded that the binding energy and the total energy curves with respect to displacements of the TM systems around the Hi, Ti and S positions support the S and Ti sites as the possible binding sites for all the systems, the magnitudes of the binding energies favoring the S center. Channeling studies however suggest that both Ti and S sites are the likely locations of Mn TM systems. We have therefore investigated the hyperfine interaction constants ( $A$ ) at both of these sites for  $Mn^0$  and  $M^{2+}$  including many-body effects which are rather important because the unpaired electrons are in d-like orbitals and have no direct contributions. Our results for  $A$  for  $Mn^0$  and  $Mn^{2+}$  when compared with experimental results [3] from Electron Paramagnetic Resonance (EPR) measurements show that the latter data can be explained with only the  $Mn^{2+}$  ion at the Ti sites, with the value for  $A$  from the  $Mn^0$  results too small to explain the EPR results. This investigation illustrates the importance of the hyperfine interactions of the TM system, together with results from channeling measurements, in deciding on the charge states and locations of the TM systems in the silicon hosts, which in turn are important for a first-principles understanding of the ferromagnetic behavior of TM systems in Silicon.

### References

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