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**First-Principles Hartree-Fock Study of Locations and Hyperfine Interactions of Transition Metal Impurities in Silicon** R.H. PINK, S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, LEE CHOW, UCF Orlando, M.B. HUANG, T.P. DAS, SUNY Albany — The study of the magnetic properties of transition metal ions in silicon is currently of great interest because of their potential applications in spintronics. An understanding of the ferromagnetism associated with the interactions between these impurities requires a knowledge of their locations in the lattice. Three possible locations of $Mn^{2+}$, $V^{2+}$, and $Cr^{+}$ ions have been investigated, namely, the interstitial hexagonal ($H_i$) and tetrahedral ($T_i$) and substitutional (S) sites. Both binding energies and hyperfine interactions are being studied using the Hartree-Fock Cluster procedure with many-body effects included by the many-body perturbation theory (MBPT) procedure. For $Mn^{2+}$ ion, the Hi site is found to be unstable while the Ti and S sites have positive binding energies. Our calculated 55Mn hyperfine constant favors the Ti site[1] which is also supported by channeling measurements.[2]

[1]G.W. Ludwig and H.H. Woodbury, Phys. Rev. Lett. 5, 98 (1960).
[2]J. LaRose and M.B. Huang (to be published).

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