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Location and Magnetic Hyperfine Properties of  $Mn^{2+}$  in Silicon. R.H. PINK, SUNY Albany, ARCHANA DUBEY, UCF Orlando, S.R. BADU, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, M.B. HUANG, SUNY Albany, LEE CHOW, UCF Orlando, T.P. DAS, SUNY Albany, UCF Orlando — Crystalline Silicon doped with the transition metal ion  $Mn^{+2}$  is ferromagnetic at room temperature and thus potentially a useful material for spintronic applications. In attempting to understand from first principles the location of  $Mn^{+2}$  and the electronic structure of the ferromagnetic system we have started work first on the dilute system. We have used the Hartree-Fock cluster procedure to determine the binding energies of the three likely locations for  $Mn^{2+}$ , substitutional (S), tetrahedral interstitial ( $T_i$ ) and hexagonal interstitial ( $H_i$ ) locations allowing for relaxation of the silicon neighbors. Our calculations show that the  $H_i$  location is unstable and the S and  $T_i$  are stable. Our nuclear magnetic hyperfine interactions results for <sup>55</sup>Mn nucleus and <sup>29</sup>Si neighbor will be presented and compared with electron spin resonance [1] experimental data.

[1] H.H. Wood bury and G. W. Ludwig Phys. Rev. <u>117</u>,102(1960)

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