**Project Title:**

# Transition Metal Impurities in Semiconductors

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I am currently investigating dilute transition metal impurities in silicon. These systems have been shown to be ferromagnetic at room temperature[1] with potential applications in spintronics[2]. I have been investigating the locations of the transition metal impurities $Mn^0$, $Mn^{2+}$, $Cr^+$ and $V^{2+}$ in silicon using the Hartree-Fock Cluster Procedure[3] combined with Many-Body Perturbation Theory[4].

The silicon lattice locations most likely to be binding sites for the transition metal ions are the tetrahedral interstitial ($T_i$), hexagonal interstitial ($H_i$), and substitutional (S) locations. As a result of my investigations, I have found that for all four impurities, the tetrahedral interstitial location in the silicon lattice is the most likely binding site. The hexagonal interstitial location, for all of the impurities, has been found to be a meta-stable saddle-point and thus not a viable candidate as the final binding location of the transition metal impurities in silicon. The substitutional location has also been found to be stable with a sizable binding energy for all three transition metal impurities; however the necessary removal of the existing silicon atom makes that location less likely as the preferred binding site. It is worth noting however that my results indicate that in silicon with preexisting vacancies this would be the most likely binding location for all three investigated transition metal impurities since it has the highest binding energy of the three previously mentioned locations for all three transition metal impurities.

By increasing the cluster size of the silicon atoms surrounding the transition metal impurities, I have found increasing stability for all of the possible binding locations in silicon. I have investigated the bonding of the neutral manganese in silicon and have found at both locations stable, but weak binding. The binding mechanism seems to be the result of a potential produced by induced dipoles in neighboring silicons by the implanted transition metal impurities. Further investigations must be made to test this hypothesis.

Over the next year I plan to continue studying the locations and spin properties of transition metal impurities in silicon. I will increase the size of the silicon clusters used to approximate the solid[3,5] to see further convergence with regards to the energy properties I've already observed. I also would like to create clusters containing pairs of transition metal impurities in order to investigate the possibility of ferromagnetism in transition metal doped silicon.

In addition to my silicon work, I have also recently investigated the Nuclear Quadrupole Interactions of the controlled substances cocaine and heroin, to establish parameters for their detection by Nuclear Magnetic Resonance methods. These controlled substance calculations have provided an excellent verification of the methods applied in my investigations of Transition Metal doped Silicon.

1. M. Bolduc, C. Awo-Affouda, A. Stollenwerk, M.B. Huang, H.G. Ramos, G. Agnello, and V.P. LaBella, Phys. Rev. B 71, 033302 (2005).

2. S.A. Wolf and D.D. Awaschalom, Science 294, 1488 (2001).

3. See for example, T.P. Das (pgs. 1-28.) in Electronic Properties of Solids Using Cluster Methods, Eds. T.A. Kaplan and S.D. Mahanti, Plenum Press, New York and London,1995.

4. N.C. Dutta, C. Matsubara, R.T. Pu and T.P. Das, Phys. Rev. Lett. 21, 1139 (1968); E.S. Chang, R.T. Pu and T.P. Das, Phys. Rev. 174, 1 (1968).

5. Nanoclusters, Volume 1: A Bridge across Disciplines (Science and Technology of Atomic, Molecular, Condensed Matter & Biological Systems), Eds. Purusottam Jena and A. Welford Castleman Jr., Elsevier, Amsterdam, New York, 2010.

## Fiscal Year 2012 List of Publications Resulting from the Use of RICC

### [Publication]

Nuclear Quadrupole Interactions in Nuclear Quadrupole Resonance Detection of Energetic and Controlled Materials: Theoretical Study; Ranjit Pati, R.H. Pink, R.H. Scheicher, Narayan Sahoo, S.N. Ray, T.P. Das; Appl Magn Reson 43, pp 591-617 (2012).