Project Title:

Transition Metal Impurities in Semiconductors

Name: ○**Roger Pink**

Laboratory at RIKEN: Advanced Meson Science Laboratory

I am 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. Furthermore, the stability of this site over other binding sites increases with larger silicon cluster approximations[5]. 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. The hexagonal interstitial location has been found to be metastable.

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 for a variety of cluster sizes 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.

In the next year I plan to create clusters containing pairs of transition metal impurities and in order to investigate the possibility of ferromagnetism in transition metal doped silicon. I will test the pair interaction of these impurities with respect to cluster size.

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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).

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