

Project Title:

Transition Metal Impurities in Semiconductors

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I am currently investigating dilute transition metal impurities in semiconductors, specifically silicon. These systems have been shown to be ferromagnetic at room temperature¹ with potential applications in Spintronics². I have been investigating the locations of the transition metal impurities Mn²⁺, Cr⁺ and V²⁺ in silicon using the Hartree-Fock Cluster Procedure³ combined with Many-Body Perturbation Theory^{4,5}. In these investigations I have had to use large clusters of silicon atoms to approximate the solid, requiring large amounts of processing time which my Quick Use account has been able to provide.

The silicon lattice locations most likely to be binding sites for the transition metal ions are the tetrahedral interstitial (Ti), hexagonal interstitial (Hi), and substitutional (S) locations. As a result of my investigations, I have found that for all three 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 metastable 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 ions.

Over the next year I plan to continue studying the locations and spin properties of transition metal impurities. In addition to the three impurities described earlier, I will investigate neutral Mn atom impurities in silicon to gain better insight into the mechanisms involved in

the binding process. My investigations seem to indicate that the binding of the transition metal impurities in silicon is a result of the transition metal impurities polarizing the surrounding neutral silicon atoms which then in turn interact with the impurity, binding the impurity to the solid. A neutral Mn atom impurity is expected to be less effective at polarizing the surrounding silicons in the lattice and consequently the neutral Mn is expected to have a lower binding energy in the silicon lattice. I also plan to increase the size of the silicon clusters used to approximate the solid^{3,6} to see further convergence with regards to the energy properties I've already observed and described above. Finally, I would like to create clusters containing pairs of transition metal impurities in order to investigate the possibility of ferromagnetism in transition metal doped silicon.

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