Project Title:

First Principles Study of Muon and Muonium in Heme Systems, Nucleic Acids, and Condensed Matter Systems

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The planned investigations proposed for 2014 on RICC are in materials science and atomic physics. We shall briefly describe our progress in the project and then describe the problems we plan to investigate in 2014.

We have continued our investigations in Transition Metal Impurities in Silicon. We have been concentrating on single TM ions in silicon, specifically Mn^0, V^{2+}, Cr^+ and Mn^{2+} in larger clusters, testing for convergence with respect to cluster size. The probable locations of the isolated ions were determined by first-principles investigations of their binding energies at different sites using Hartree-Fock theory[1] combined with many-body perturbation theory. From this procedure it was found that the binding energies for V^{2+} and Mn^{2+} ions were largest for the S_v site, followed by the T_i site and then the H_i. For Cr^+ ion, the binding energies were found to be positive for the H_i and T_i sites but an order of magnitude smaller than for Mn^{2+} and V^{2+} ions, with the binding energy for the S_v site very close to zero. For Mn^0 atom, both H_i and T_i sites are unstable with negative binding energy, only the S_v site being stable with positive binding energy. For Mn^{2+} ion, channeling data in Silicon have shown that while the T_i site is the most abundant site for the Mn^{2+} ion, the S_v site also can be present. The observed greater abundance of the T_i site for Mn^{2+} in silicon over the S_v site can perhaps be explained by the fact that while the T_i site available in pure silicon, the S_v site requires the presence of substitutional vacancies with low formation probability when the vacancy concentration is low. There was noticeable convergence for these results with respect to cluster size.

The next paragraph describes our plans for research using the RIKEN Supercomputer TM-Silicon system for the year 2014.

Our plans for the year 2014 are to proceed with our investigations to study the interactions between pairs of neighbors of theses paramagnetic atomic and ionic systems. To first find the stable locations of the pairs and then the energy differences between the pairs and the corresponding two isolated ions to see whether the pairs are ferromagnetic, antiferromagnetic or paramagnetic.

We will investigate the possibility of ferromagnetic or antiferromagnetic couplings of Mn^{2+}-Mn^{2+}, Mn^{2+}-Mn^0 and Mn^0-Mn^0 pairs in silicon. The discrepancy between predicted hyperfine constant for ^{55}Mn for a single Mn^0 in silicon and the measured ^{55}Mn hyperfine constants for the dilute Mn-Si system suggests that free Mn^0 may not be present in dilute Mn-Si system. However in less dilute Mn-Si systems, it is possible that Mn^{2+} - Mn^0 and Mn^0-Mn^0 pairs could be stable. This is why we will study all three pairs involving Mn^{2+} and Mn^0 that we have mentioned earlier will be investigated. We will investigate both the stabilities of the three molecular pairs in silicon by studying the total energies of both the molecular pairs in the cluster systems chosen for our investigation as well as the cluster for the single atom or ion in silicon. The basis sets found to provide best agreement with the ^{55}Mn experimental hyperfine constant in dilute systems will be used for the molecular systems. We shall initially study the Mn^{2+}-Mn^{2+} pair because for the dilute system Mn^{2+}-silicon the hyperfine constants, from our earlier theoretical investigations, agrees well with EPR results. For the Mn^{2+}-Mn^{2+} pair investigation, we shall study all the nine possibilities corresponding to each two Mn^{2+} ion being in any of the three positions H_i, T_i and S_v. Relaxation in the positions of the Mn^{2+} ions, and the silicon atoms in the cluster corresponding to the Mn^{2+}-Mn^{2+} pair in silicon, will be included in the investigation. Both the stabilities of the pairs from the energy results and the ferromagnetic, paramagnetic or antiferromagnetic behaviors, from the spin density distributions and spin-populations on the Mn^{2+} ions will be examined. Subsequently, similar investigations will be carried out for Mn^{2+}-Mn^0 and Mn^0-Mn^0 pairs.

1. T.P. Das, T.A. Kaplan, S.D. Mahanti, editors. Electronic Properties of Solids Using Cluster Methods. New York: Plenum Press; 1995. P. 1-28