Prasenjit Sen

Research Summary:

My main research activity during this period has been to understand structural, electronic and magnetic properties of small bi-metallic clusters. The particular system we have focussed on is $3d$ transition metal (TM) doped sodium clusters. Recently it has been claimed that small TM doped Au clusters have large magnetic moments. On general chemical arguments we predicted that TM doped small alkali metal clusters of same size will have larger magnetic moments. This led us to do detailed first-principles electronic structure calculation of these clusters. Our calculations show that indeed these clusters have large moments. What is surprising is that early TM (Sc, Ti and V) doped Na_5 and Na_6 clusters have moments that are larger than the moments on the corresponding isolated TM atoms. It turns out that a large overlap of TM d and Na s states lead to larger occupancy of d-type states compared to isolated TM atoms in the early TM series. This leads to an enhancement of the moment on the TM atoms in these clusters. It is interesting to note that there is no such s-d overlap in TM-Au_6 clusters, and hence the corresponding moments are also smaller.

A second problem that I have worked on in collaboration with Prof. G. P. Das of the IACS, Kolkata and his group is to search for Si-based nano-cluster systems suitable for hydrogen storage. In the process we have discovered through first-principles calculations that a $Si_{60}H_{60}$ cluster forms a (meta)-stable, highly symmetric fullerene structure. This is very surprising in view of the well-known fact that pure Si_{60} does not form fullerene structure, unlike C_{60}. We are now studying hydrogen storage on Ti atoms attached to the pentagonal faces of the $Si_{60}H_{60}$ fullerenes.

Another problem I have worked on is to study magnetic properties on alkali metal dioxide solids, in collaboration with Dr. Priya Mahadevan of the SNBNCBS, Kolkata. First-principles calculations based density functional theory (DFT) within local spin-density approximation (LSDA) predict that solid KO_2 has a ferromagnetic ground state. This is surprising in view of that fact that there are no elements with unfilled d or f shells in this compound. In order to be convinced that result not an artifact of LSDA (though LSDA, in general, reduce spin polarization), we did *ab initio* quantum Monte Carlo (QMC) calculations for the electronic structure of this solid. QMC methods work with correlated wavefunctions, and usually reproduce/predict properties of materials much more accurately. To our surprise, QMC calculations also predict KO_2 solid to have a ferromagnetic ground state. We are now in the process of understanding the microscopic origin of this unusual ferromagnetism.

Publications:

1. Prasenjit Sen, *Peierls instability and electron-phonon coupling in a one-dimensional sodium wire,* Chemical Physics Letters **428**, 430, (2006)

Preprints:

1. Kalpataru Pradhan and Prasenjit Sen, *Unexpectedly large moments on TM@Na_n clusters: (TM=Sc, Ti, V; $n = 5, 6$),*

Conference/Workshops Attended:

1. *Workshop on Computational Materials Theory*, India, July, 2006.
2. *Materials Modeling at Different Length Scales*, India, October 2006.

Visits to other Institutes:

1. Indian Association for the Cultivation of Science, Kolkata, India, April 2006.
2. IACS, Kolkata, India, December 2006.
3. S. N. Bose National Center for Basic Sciences, Kolkata, India, March 2007.

Invited Lectures/Seminars:

1. *Peierls instability and electron-phonon coupling in a one-dimensional sodium wire*, Materials Modeling at Different Length Scales, DAE-BRNS, BARC, Mumbai, October 2006.

Other Activities:

1. I have been acting as the contact person for HRI in the National Grid Initiative (Garuda).
2. I organized a set of lectures for the VSP students in condensed matter physics during the summer of 2006. I was also one of the speakers. I advised two students – Kinjal Das Biswas (IITK) and Varada Bal (IIT-Kgp) for their VSP projects.
3. I taught a course on Numerical Methods during the Aug-Dec semester, 2006.