Kalpataru Pradhan

Research Summary:

1. Extending our previous work on Kondo Lattice Model (KLM), we focus on intermediate coupling regime where neither the perturbative RKKY approach nor double exchange is valid. We are able to uncover the planar spiral states, A and C type of antiferromagnetic order along with ferromagnetic and G type antiferromagnetic order accompanied by phase separation between different phases using variational calculations. Using full spin-fermion Monte Carlo (Traveling Cluster Approximation), we also map out the ground state and estimate the ordering temperature, transport properties and spectral features of the model. We discuss our results in the context of the 'heavy rare earth' 4f elements, which are class of materials with 'large S' magnetic moments coupled to 5d-6s conduction electrons via exchange interaction. The systematic increase of the 4f spin from Yb to Gd can be mapped out on to a variation of the effective exchange in our classical KLM and we suggest that these metals involve physics well beyond the RKKY interaction regime as one moves from Yb to Gd in rare earth family.

2. The complicated interplay of spin, charge, lattice and orbital degrees of freedom is believed to induce unexpected magnetic and transport phenomena in manganese oxides of the form (R,A)BO_3 (R for Rare Earth Element, A for Alkaline Earth Element and B for Manganese). The difference between A and B site disorder holds a key to the phase separation and spatial inhomogeneity in the manganites. In half doped manganites with A type disorder, with randomly placed R and A elements, converts the CO-OO-CE-I (Charge Order-Orbital Order-Zigzag pattern of ferromagnetic chains-Insulator) to a short range correlated glass. But the substitution of Mn by few percents of Cr or Ru (B site disorder) leads to metalicity with coexistence of FM-M (Ferromagnetic Metal) and CO-OO-AF-I domains. We study a two orbital double-exchange model in two dimensions in the presence of antiferromagnetic superexchange, Jahn-Teller Coupling and substitutional disorder. We compare the impact of weak homogeneous disorder to that of a low density of strong scatterers on CO-OO-CE-I at half doping. Even moderate homogeneous disorder suppresses the CO-OO-CE phase and leads to glass which is more or less a strong insulator with nano scale correlations. Dilute strong scatterers of comparable strength leads to coexistence of FM-M and CO-OO-AF clusters. This in turn lead to metalicity. It also seems that magnetic character of the B site impurity plays a important role at different doping.

3. In search of clusters with large magnetic moments, we dope transition metals (TM) to the Na clusters (motivated from large magnetic moments on TM doped with small gold clusters). Our central focus is to find ground state atomic,electronic structures and most importantly magnetic moments of Sc, Ti, V on small size Na clusters of size n (n=5,6) using Density Functional Theory (DFT). Interestingly we found Ti@Na_n and V@Na_n posses large magnetic moments, larger than atomic moments of Ti and V respectively. The origin of such unusual large magnetic moments is due to large overlap of Na s and TM d orbitals, and the relative values of electronegativity of the Na and TM atoms. We also find large magnetic moments with other TM like Cr, Mn and Fe doping in these clusters. We are doing a systematic size dependent analysis of Na clusters doped with different TM.

Preprints:

1. Kalpataru Pradhan and Pinaki Majumdar, *The classical Kondo Lattice at intermediate Coupling* (preprint)
2. Kalpataru Pradhan and Pinaki Majumdar, *Magnetism Beyond RKKY Interaction: Revisiting the 4f Metals* (preprint)
3. Kalpataru Pradhan and Prasenjit Sen, *Unexpectedly large magnetic moments on TM@Na_n clusters (TM=Sc,Ti,V; n=5,6)* (preprint)
4. Kalpataru Pradhan, Anamitra Mukherjee and Pinaki Majumdar, *The distinct Effect of Homogeneous Weak Disorder and Dilute Strong Scatterers on Phase Competition in the manganites* (preprint, Submitted to PRL)

Conference/Workshops Attended:

1. *Summer School on Electronic Structure Methods and their Applications, and Worksh on Computational Materials theory*, Bangalore,India, 10-22 July 2006.
2. *International Conference on Physics Near The Mott Transition*, Bangalore,India, 24-28 July,2006.
3. *Workshop on Correlated Systems and Novel Materials*, Kharagpur,India, 16-18 January,2007.

Other Activities:

1. Condensed Matter talk on *The Kondo lattice with classical spins: magnetism, transport and dilution effects*
2. Condensed Matter talk on *Hypothetical Zincblende Structure of MnAs: A Density Functional Calculation*