Electronic structure and magnetism in low dimensional and cluster assembled solids.

Indra Dasgupta
Department of Solid State Physics and Center for Advanced Materials
Indian Association for the Cultivation of Science
Jadavpur
Kolkata 700 032

We shall analyze the electronic structure of low dimensional and cluster assembled solids exhibiting novel magnetic properties. As a first example we shall explain the electronic structure of the spin gap compound Sr2Cu(BO3)2 [1] and illustrate that a careful analysis of the electronic structure plays a key role for the identification of the correct low energy model Hamiltonian for this system. The validity of the model is checked by calculating the magnetic susceptibility as a function of temperature and magnetization both as a function of temperature as well as field using quantum Monte Carlo technique and comparing them with the available experimental data. This comparison establishes the suitability of the coupled dimer model for the description of the low energy physics of Sr2Cu(BO3)2. Next we shall present a detailed study of the magnetic properties of unique cluster assembled solids namely Mn doped Ge46 and Ba8Ge46 clathrates [2]. We find that ferromagnetic (FM) ground states may be realized in both the compounds when doped with Mn. In Mn2Ge44, ferromagnetism is driven by hybridization induced negative exchange splitting, a generic mechanism operating in many diluted magnetic semiconductors. However, for Mn-doped Ba8Ge46 clathrates incorporation of conduction electrons via Ba encapsulation results in RKKY-like magnetic interactions between the Mn ions. The RKKY mechanism also provide a natural explanation to the experimental results available for Ba8Mn2Ge44 clathrate.

[1] Jayita Chakraborty and Indra Dasgupta, Phys. Rev B 86. 054434 (2012)
[2] N. Ganguli, K.V. Shanavas and I. Dasgupta, Journal of Physics: Condensed Matter 24 (50), 505501, (2012)