Title of the Thesis: ***Electronic structure calculations and microscopic understanding of strongly correlated systems***

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Abstract:

It is essential to discover materials with improved properties for technologies are becoming materials limited i.e., novel materials are a key to new technologies. It is beyond surprise that modeling is playing an ever increasing vital role to find out new materials. Properties of novel materials in microscopic terms can be best understood with the help of material specific theory, especially computational theory.

The behavior of low-dimensional strongly correlated systems (SCS), that we are interested in, is dominated by zero-point spin fluctuation. As a consequence, they show a variety of interesting magnetic properties which are not present in their classical counterparts. Interest in quantum spin systems has been driven by the importance for understanding the mechanism of high-T_c superconductivity and in recent years its probable application in the field of quantum computation.

A very important aspect in the study of SCS is the knowledge of the spin model, given a specific compound. A microscopic investigation for this purpose is essential, since often the nature of the underlying exchange network is not what is expected from crystal structure-one need to take into account the chemistry aspect. Microscopic investigation also provides with quantitative numbers corresponding to various exchange interactions. Another possible route often used, is to fit the measured susceptibility data with some assumed theoretical model. This method suffers from drawback that the susceptibility data is quite insensitive to the details and two different models may be fitted to same data with two different set of fitting parameters. $(VO)_2P_2O_7$ forms a classic example in this regard which turned out to be an alternating chain compound while it was originally considered to be an example of ladder compound. Therefore microscopic understanding is required for the sake of uniqueness.

In the thesis, we aim on deriving spin model Hamiltonians out of full LDA-DFT calculations considering a variety of systems belonging to the category of strongly correlated systems.