

**Stony Brook University
The Graduate School**

Doctoral Defense Announcement

Abstract

Realistic Theoretical Study of Long-Range Order in
Half-Doped Manganites

By

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The exploration of distinct orders and their mutual interplay in systems with transition metal elements is of significant importance to condensed matter physicists, as these orders may provide a way to tune material properties, giving rise to a wide practical application of these materials in industry.

Manganese oxides, such as $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ have attracted considerable attention due to the observed colossal magnetoresistance effect (CMR) at certain levels of doping. Both the origin and stability of these systems as well as the role of leading mechanisms are currently under great debate in the literature. To gain deeper microscopic insight on the issue, we developed novel, three-step approach within Wannier states framework, that allows one to map out most relevant mechanisms and evaluate their relative importance for the stability of the ground state. This approach allows natural solution of current puzzle of weak charge disproportion experimentally observed in half-doped manganites with traditional $\text{Mn}^{3+}/\text{Mn}^{4+}$ picture.

Finally, we explore the possibility of using biorthogonal wavelet basis set in density functional calculations.

Date: December 04, 2007

Time: 9.00 am

Place: (Physics Building, D-122)

Program: Physics

Dissertation Advisor: Prof. Wei Ku