

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic, structural and magnetic properties of LaMnO₃ phase transition at high temperature PABLO RIVERO, Louisiana State University, VINCENT MEUNIER, Rensselaer Polytechnic Institute, WILLIAM SHELTON, Louisiana State University — We have developed a theoretical approach for investigating systems that contain a range of correlation that varies with experimentally controlled parameters. We applied this method to the LaMnO₃ compound[1,2,3] to accurately describe the antiferromagnetic (AFM) insulating ground-state, the metal-to-insulator transition and the high temperature ferromagnetic (FM) state, where we observe a half-metallic behavior. [1]: T. Saitoh, A. E. Bocquet, T. Mizokawa, H. Namatame, A. Fujimori, M. Abbate, Y. Takeda, and M. Takano, *Phys. Rev. B*, , 13942 (1995). [2]: J. S. Zhou, and J. B. Goodenough, *Phys. Rev. B*, , R15002 (1999). [3]: J. Rodriguez-Carvajal, M. Hennion, F. Moussa, A. H. Moudan, L. Pinsard, and A. Revcolevschi, *Phys. Rev. B*, , R3189 (1998).

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Date submitted: 06 Nov 2015

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