MAR12-2011-003655

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Covalency, Excitons, Double Counting and the Metal-Insulator Transition in Transition Metal Oxides

XIN WANG, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park

We present single-site dynamical mean-field studies of realistic models of transition metal oxides, including the cuprate superconductors and rare earth nickelates (in bulk and superlattice form). We include orbital multiplet effects and hybridization to ligands. We explicitly calculate the d-d exciton spectra for cuprates, finding sharp exciton lines in both metallic and insulating phases, which should be visible in experiments. We also find that the additional $d_{3z^2-r^2}$ orbital does not contribute to an additional Fermi surface at any reasonable doping, in contradiction to previous slave-boson studies. The hybridization to ligands is shown to have crucial effects, for example suppressing the ferro-orbital order previously found in Hubbard model studies of nickelates. Hybridization to ligands is shown to be most naturally parametrized by the d-orbital occupancy. For cuprates and nickelates, insulating behavior is found to be present only for a very narrow range of d-occupancy, irrespective of the Coulomb repulsion. The d-occupancy predicted by standard band calculations is found to be very far from the values required to obtain an insulating phase, calling into question the interpretation of these materials as charge transfer insulators.

This work is done in collaboration with A.J. Millis, M.J. Han, C.A. Marianetti, L. de' Medici, and H.T. Dang, and is supported by NSF-DMR-1006282, the Army Office of Scientific Research, and the Condensed Matter Theory Center and CNAM at University of Maryland.

[1] X. Wang, H. T. Dang, and A. J. Millis, Phys. Rev. B 84, 014530 (2011).
[2] X. Wang, M. J. Han, L. de' Medici, C. A. Marianetti, and A. J. Millis, arXiv:1110.2782.
[3] M. J. Han, X. Wang, C. A. Marianetti, and A. J. Millis, Phys. Rev. Lett. 107, 206804 (2011).