Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Sorting Category: 05.4 (T)

Charge and Spin Ordering in Insulator $Na_{0.5}CoO_2$: Effects of Correlation and Symmetry KWAN-WOO LEE, WARREN PICKETT, University of California, Davis — The discovery by Takada and coworkers of superconductivity in $Na_{0.3}CoO_2 \bullet 1.3\ H_2O$ near 5K has led to extensive studies of the rich variation of properties in the Na_xCoO_2 system ($0.2 \leq x \leq 1$), which has a triangular lattice of Co sites and a layered structure. In addition, specifically at x=0.5, the system has been observed to undergo a charge disproportionation ($2Co^{3.5+} \rightarrow Co^{3+}+Co^{4+}$) and metal-insulator transition at 50 K, while the rest of the phase diagram is metallic. We will present results of studies of charge disproportionation and charge- and spin-ordering in insulating in $Na_{0.5}CoO_2$, applying ab initio band theory including correlations due to intra-atomic repulsion. Various ordering patterns (zigzag and two striped) for four-Co supercells are analyzed before focusing on the observed "out-of-phase stripe" pattern of antiferromagnetic Co^{4+} spins along charge-ordered stripes. This pattern relieves frustration and shows distinct analogies with the cuprate layers: a bipartite lattice of antialigned spins, with axes at 90° angles. Substantial distinctions with cuprates are also discussed, including the tiny gap of a new variant of "charge transfer" type within the Co 3*d* system. [References] [1] K. Takada et al., Nature **422**, 53 (2003). [2] M. L. Foo et al., Phys. Rev. Lett. **92**,247001 (2004). [3] K.-W. Lee, J. Kunes, P. Novak, and W. E. Pickett, Phys. Rev. Lett. **94**, 026403 (2005). [4] K.-W. Lee and W. E. Pickett, cond-mat/0510555.

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Date submitted: 24 Nov 2005 Electronic form version 1.4