Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-principles determined charge and orbital interactions in Fe_3O_4[1] FEI ZHOU, UCLA, GERBRAND CEDER, MIT — In this work we have attempted to describe the charge and orbital degrees of freedom in fo with a classical effective energy model. Electronic and lattice effects are both included through first-principles calculated energies from which the model is parametrized. The calculated charge and orbital interactions in fo are found to be physically meaningful. The energy landscape is complex in terms of frustrated charge and orbital interactions as well as their competition. Additionally, although our predicted ground state structure has smaller periodicity than experimentally observed, it reveals the possibility that not only charge and orbital ordering, but the Jahn-Teller lattice distortions may also decide the structure. Therefore this work may help better understand the problem of the low-T magnetite structure. Beyond magnetite, our approach can be easily adapted to explore other transition metal oxides where charge and/or orbital order exist.

[1]This work is supported by DOE under contract DE-FG02-96ER45571, and in part by NSF through the National Partnership for Advanced Computing Infrastructure using SDSC Datastar. FZ thanks Dr. C. Fischer for his help in data analysis.

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Date submitted: 26 Nov 2008 Electronic form version 1.4