Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Designing ferromagnetism in early transition metal oxides in bulk and superlattice forms[1] HUNG DANG, ANDREW MILLIS, Department of Physics, Columbia University — The circumstances under which early transition metal oxides could exhibit ferromagnetism are determined using density functional plus single-site dynamical mean field methods. Particular attention is paid to the consequences of the $GdFeO_3$ distortion and other octahedral rotations. Ferromagnetism is favored by the combination of intermediate carrier concentration (formal valence $\sim d^{1.5}$) and large tilt angle. The decrease of $GdFeO_3$ distortion amplitude with hole doping away from d^2 is shown to keep the bulk solid solution $La_{1-x}Sr_xVO_3$ outside of the ferromagnetic regime. In superlattices such as $(LaVO_3)_m(SrVO_3)_1$, carrier concentration and tilt angle may be decoupled, potentially enabling ferromagnetism as suggested by experiment[1].

[1] U. Lüders, W. C. Sheets, A. David, W. Prellier, and R. Frésard, Phys. Rev. B 80, 241102(R) (2009).

[1]Supported by the Basic Energy Sciences Program of the US Department of Energy under grant DOE ER046169.

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Date submitted: 06 Nov 2012 Electronic form version 1.4