Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Magnetic States of the Two-Leg Ladder Iron Selenides QINLONG LUO, ANDREW NICHOLSON, JULIAN RINCON, SHUHUA LIANG, ADRIANA MOREO, ELBIO DAGOTTO, Univ. of Tennessee/ORNL, JOSE RIERA, Universidad Nacional de Rosario, GONZALO ALVAREZ, ORNL, LIMIN WANG, WEI KU, BNL — Neutron scattering experiments have unveiled a dominant spin arrangement in the two-leg ladder selenide compound $BaFe_2Se_3$, involving ferromagnetically ordered 2×2 iron-superblocks, that are antiferromagnetically coupled among them (the "block-AFM" state). Our numerical study of the electronic five-orbital Hubbard model, within the Hartree-Fock approximation and using first principles techniques for the hopping amplitudes, has shown that the exotic block-AFM state is indeed stable at realistic electronic densities $n \sim 6.0$. Another state with wavevector $(\pi, 0)$ becomes stable in other portions of the phase diagrams, including $n \sim 5.5$, as found experimentally in KFe_2Se_3. In addition, our study unveils several competing magnetic phases that could be experimentally stabilized varying either n chemically or the electronic bandwidth by pressure. Similar results were obtained using two-orbital models, studied here via Lanczos and DMRG techniques [1]. [1] Qinlong Luo, et al, arXiv: 1205.3239, and references therein.

Qinlong Luo
Univ. of Tennessee/ORNL

Date submitted: 09 Nov 2012 Electronic form version 1.4