Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Biquadratic and ring exchange interactions in orthorhombic perovskite manganites NATALYA FEDOROVA, CLAUDE EDERER, NICOLA SPALDIN, Materials Theory, ETH Zurich, ANDREA SCARAMUCCI, Laboratory for Developments and Methods, Paul Scherrer Institut — We use ab initio electronic structure calculations within the GGA+U approximation to density functional theory (DFT) to determine the microscopic exchange interactions in the series of orthorhombic rare-earth manganites (o-$RMnO_3$). Our motivation is to construct a model Hamiltonian (excluding effects due to spin-orbit coupling), which can provide an accurate description of the magnetism in these materials. First we map the exchange couplings for several representatives of o-$RMnO_3$ series onto a Heisenberg Hamiltonian and find a clear deviation from the Heisenberg-like behavior. We demonstrate that this deviation can be explained only by the presence of relatively strong higher order exchange interactions (biquadratic and four-spin ring couplings) and show that they have the strongest effect in compounds, where nearest-neighbor exchange interactions are weakened due to the presence of large $GdFeO_3$-type distortion. Finally we discuss how these higher order terms determine magnetic ground states, influence magnetic excitations and define the multiferroic properties of o-$RMnO_3$.

Natalya Fedorova
Materials Theory, ETH Zurich

Date submitted: 06 Nov 2015 Electronic form version 1.4