Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Microscopic modeling of the 3D quantum magnet Cu_2OSeO_3
OLEG JANSON, MPI CPfS, Dresden, Germany, IOANNIS ROUSOCHATZAKIS, ULRICH ROESSLER, JEROEN VAN DEN BRINK, IFW Dresden, Germany, ALEXANDER TSIRLIN, HELGE ROSNER, MPI CPfS, Dresden, Germany — Unlike most undoped cuprates, the $S = 1/2$ Heisenberg magnet Cu_2OSeO_3 exhibits a ferrimagnetic ground state and sizable magnetoelectric coupling. Recent experiments reported magnetic-field-induced emergence of skyrmions in this material. Based on extensive DFT band structure calculations we evaluate the microscopic magnetic model, including isotropic (Heisenberg) and anisotropic (Dzyaloshinskii-Moriya) terms. We extract five relevant couplings that form a complex, but non-frustrated spin model which can be described as a pyrochlore lattice of magnetic tetrahedra. A peculiar feature of this lattice is the alternation of "strong" (the constituent spins are strongly coupled) and "weak" tetrahedra. Profiting from a separation of the energy scales we develop an effective model, treating strong tetrahedra either as a classical $S = 1$ object or as a coherent quantum superposition of classical states. For the latter case, we find an excellent agreement with the quantum Monte Carlo simulations of the full model and the experimental magnetization and neutron diffraction data. Quite surprising for a 3D model we find distinct manifestations of quantum fluctuations. The developed effective model can be further used to model the field-induced behavior including the formation of skyrmions.

Helge Rosner
Max Planck Institute for Chemical Physics of Solids, Dresden

Date submitted: 11 Dec 2012 Electronic form version 1.4