Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Exchange constants and spin waves of MnV_2O_4 from first principles DFT calculations RAVINDRA NANGUNERI, SERGEY SAVRASOV, University of California, Davis — We present results of DFT calculations of exchange constants of the magnetic spinel MnV_2O_4. The starting point is the one-particle eigenfunctions of the Kohn-Sham auxiliary Hamiltonian as a function of the self-consistent, converged charge density. Using linear response and perturbation theory, the exchange constants between the magnetic ions Mn and V are calculated in both the collinear and non-collinear, orbital-ordered phases of the spinel. The collinear exchanges have exchange constants proportional to the unit matrix, which means they are isotropic. On the other hand, the non-collinear exchanges have unequal diagonal elements and in addition have off-diagonal elements, revealing anisotropic magnetic interactions. The anisotropy is traced to the orbital-order and non-collinear spin structure of the low-temperature ground-state. We find that the interactions between the V atoms can sometimes be anti-ferromagnetic. The V atoms are located at the vertices of a corner-sharing tetrahedral lattice, commonly known as a pyrochlore lattice. AFM interactions on such a lattice are geometrically frustrated because all pair-wise bond energies cannot be simultaneously minimized with a classical spin configuration. It has been experimentally found that as the temperature is lowered, MnV_2O_4 undergoes a transition from a paramagnet with a cubic symmetry structure phase to a ferrimagnetic with cubic symmetry phase at 56 K.

Ravindra Nanguneri
University of California, Davis

Date submitted: 27 Nov 2010 Electronic form version 1.4