Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Long-range antiferromagnetic interactions in ZnFe$_2$O$_4$ and CdFe$_2$O$_4$[1] CHING CHENG, Department of Physics, National Cheng Kung University, Tainan, Taiwan , CHING-SHENG LIU, Yi-Jia Junior High School, Luzhu Shiang, Kaohsiung County 82143, Taiwan, HSUEH FANG YEH, Department of Physics, National Cheng Kung University, Tainan, Taiwan — For the first time, the Fe-Fe interactions in the well known geometrically frustrated antiferromagets of Zinc and Cadmium ferrite are determined quantitatively by considering structures of different collinear magnetic distributions using first-principles methods. Both the generalized gradient approximation (GGA) and GGA plus the onsite Coulomb interaction (GGA+U) are considered for the exchange-correlation energy functional. The interactions up to third neighbors are determined to be all antiferromagnetic regardless of which approximation scheme (GGA or GGA+U) is used. Surprisingly, the third neighbor interaction is much stronger than the second-neighbor one. The magnetic distributions have prominent effects on energies as well as density of states, including band gaps, for both normal and inverse spinel structures of these two materials. The possible magnetic distributions coincident with neutron scattering results are also investigated.

Ching Cheng
Department of Physics, National Cheng Kung University, Tainan, Taiwan

Date submitted: 24 Nov 2008   Electronic form version 1.4