Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Ferromagnetic versus helical order in edge sharing CuO_2 chains - a computational study HELGE ROSNER, Max Planck Institute for Chemical Physics of Solids Dresden, Germany, ULRIKE NITZSCHE, Leibniz Institute for Solid State and Materials Research Dresden, ALEXANDER TSIRLIN, Max Planck Institute for Chemical Physics of Solids Dresden, Germany, ROMAN KUZIAN, STEFAN-LUDWIG DRECHSLER, Leibniz Institute for Solid State and Materials Research Dresden — The magnetic ground state of edge sharing CuO_2 spin 1/2 Heisenberg chains with nearest neighbor exchange J_1 and second neighbor exchange J_2 depends delicately on structural details of the crystal structure, like Cu-O-Cu bond angles, Cu-O distances and the position of the cations. Without taking into account a renormalization by the interchain coupling, a critical ratio $\alpha = -J_2/J_1$ separates a ferromagnetic from a helical ground state (FM for $\alpha < 1/4$, helical for $\alpha > 1/4$). Here, we present a density functional based band structure study that investigates the different influences of various structural parameters for Li_2CuO_2 as example compound. We find that the ferromagnetic and antiferromagnetic contributions develop rather differently for the same structural changes. Therefore, the key parameter α for the ground state is especially sensitive for small structural changes that might be induced by temperature or pressure variation.

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

Date submitted: 09 Nov 2011 Electronic form version 1.4