Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Orbital Ordering in Cs_2AgF_4 - an electronic structure study
DEEPA KASINATHAN, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, KLAUS KOEPERNIK, IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany; Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, ULRIKE NITZSCHE, IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany, HELGE ROSNER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — The argentate Cs_2AgF_4, first synthesized in 1974 has many similarities to the high-T_c cuprates, featuring AgF_2 sheets in place of CuO_2 sheets. While the undoped cuprates are antiferromagnetic, this argentate is ferromagnetic with a T_{Curie} of about 15 K. Density functional calculations in the proposed tetragonal structure produce an itenerant half-metallic ferromagnet. Recent inelastic neutron scattering experiments have suggested an orthorhombic structure that allows an orbitally ordered ferromagnetic ground state. We performed electronic structure calculations using the LDA+U method on this system and were able to obtain an orbitally ordered ground state, not only for the newly proposed orthorhombic lattice but also for the orginal tetragonal lattice by constraining the bravais lattice and allowing the change of the atomic basis. In specific, very small changes in the position of the in-plane fluorine atoms already trigger an orbital ordering. Our calculated energy scale shows that this orbitally ordered state should be stable for all temperatures, consistent with the experiment.

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Date submitted: 21 Nov 2006 Electronic form version 1.4