

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Quasi one-dimensional magnetism driven by unusual orbital ordering in CuSb_2O_6 ¹ HELGE ROSNER, DEEPA KASINATHAN, KLAUS KOEPERNIK, Max Planck Institute for Chemical Physics of Solids Dresden, Germany — Cuprate compounds, including the family of high-Tc-superconductors, exhibit a large variety of exotic physical properties. This variety is determined by the interplay of different interactions; mainly covalency, ligand-fields and strong correlation effects. A nearly universal component of cuprate systems is a strongly elongated CuO_6 -octahedron wherein the exotic behaviour finds its origin in the deceptively simple planar Cu-O orbital lying in its basal plane. In this well established standard scenario, the involvement of the apical out-of-plane orbitals is not settled completely. The surprisingly regular CuO_6 -octahedra of CuSb_2O_6 offer a unique opportunity to elucidate this scenario due to the changed balance of interactions in this system. We present an electronic structure study resulting in an hitherto unobserved ground state originating from a competition of in- and out-of-plane orbitals. Our results show that strong Coulomb correlation drives a surprising and unique orbital ordering. This, gives rise to an unusual and strongly one-dimensional magnetic ordering that is unlike any ordering observed in conventional low-dimensional cuprates. Our results provide a unique and natural interpretation of recent neutron data.

¹Finacial support from the Emmy-Noether-Programm is acknowledged.

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Date submitted: 17 Nov 2006

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