Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Semimetallic Antiferromagnetism in the Half-Heusler Structure: CuMnSb TAE SEONG JEONG, UC-Davis, RUBEN WEHT, CNEA, WARREN PICKETT, UC-Davis — The half-Heusler compound CuMnSb, the first antiferromagnet in the Mn-based class of Heuslers and half-Heuslers that contains several conventional and half metallic ferromagnets, shows a peculiar stability of its magnetic order in high magnetic fields. Density functional based studies reveal an unusual nature of its unstable (and therefore unseen) paramagnetic state, which for one electron less (CuMnSn or NiMnSb, for example) would be an (accidental) zero gap semiconductor between two sets of very flat, topologically separate bands of Mn $3d$ character. The extremely flat and narrow Mn bands result from the environment, which has four tetrahedrally coordinated Cu atoms whose $3d$ states lie well below the Fermi level and four other tetrahedrally coordinated empty sites. The AFM phase can be pictured as a heavily doped $Cu^{1+}Mn^{2+}Sb^{3-}$ compensated semimetal with heavy mass electrons and light mass holes. The ratio of the linear specific heat coefficient and the calculated Fermi level density of states indicates a large mass enhancement $m^*/m \sim 10$.

Tae Seong Jeong
UC-Davis

Date submitted: 04 Dec 2004 Electronic form version 1.4