

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Band structure and Fermi surface of  $\text{Ba}_2\text{Ca}_3\text{Cu}_4\text{O}_8\text{F}_2$**  WENHUI XIE, OVE JEPSEN, OLE K. ANDERSEN, Max-Planck-Institut FKF Stuttgart Germany, ZHI-XUN SHEN, Stanford University — Recently Y. Chen *et al.* have measured the Fermi Surface (FS) of the fluorinated four  $\text{CuO}_2$  layer superconductor,  $\text{Ba}_2\text{Ca}_3\text{Cu}_4\text{O}_8\text{F}_2$ , using angular resolved photoemission spectroscopy (ARPES). Surprisingly, they found only two large  $(\pi,\pi)$  centered hole FS sheets, while four would have been expected. In order to investigate the reason for this we have performed first-principles electronic band structure calculations for this compound. As expected four antibonding copper-oxygen bands cross the Fermi level of which the two have dominantly orbital character on the two inner-layers and the other two have most orbital character on the outer-layers. The splitting between these bands is, however, much smaller than the splitting between the two measured FS sheets. The fluorine were claimed to replace all apical oxygens, however, by partly substituting apical oxygen as well as oxygen in the four  $\text{CuO}_2$  layers by fluorine, good agreement with the experimental FS could be obtained.

Ove Jepsen  
Max-Planck-Institut FKF Stuttgart

Date submitted: 15 Dec 2005

Electronic form version 1.4