Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Strong orbital-dependent d-band hybridization and Fermi surface reconstruction in metallic $Ca_{2-x}Sr_xRuO_4$[1] EUNJUNG KO, Department of Physics and IPAP, Yonsei University, Seoul, Korea, B. J. KIM, School of Physics and CSCMR, Seoul National University, Seoul, Korea, C. KIM, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Seoul, Korea — The layered ruthenate $Ca_{2-x}Sr_xRuO_4$ displays diverse ground states ranging from a superconductor (x=2) to a Mott insulator (x=0), accompanied by structural distortions.We investigate the effects of RuO_6 rotation on Ru 4d band structures in the metallic phase ($0.5<x<2$) by first-principles electronic structure calculations. Our study reveals that the symmetry lowering due to RuO_6 rotation induces a strong orbital-dependent t_{2g}- e_g hybridization. As a result, only the d_{xy} band among three t_{2g} bands is severely affected and thereby the Fermi surface is reconstructed, forming a new electron-like d_{xy} Fermi surface near Γ and nested sections near x=0.5. These findings should provide a new insight on the electron correlation in the material.

[1]This work is supported by the BK21 Project.Computational resource is provided by KISTI under the 7th Strategic Supercomputing Support Program.

Hyoung Joon Choi
Department of Physics and IPAP, Yonsei University, Seoul, Korea

Date submitted: 20 Nov 2006 Electronic form version 1.4