

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Orbital-Resolved Soft X-ray Spectroscopy Measurements of Sr_2RuO_4 Electronic Structure. TIM SCHULER, MPT Polymers, J. HOOPER, Tulane University, ZHIQIANG MAO, Tulane University, DAVID EDERER, Tulane University, GUO-PING ZHANG, Indiana State University, TOM CALLCOTT, University of Tennessee — Strontium ruthenate (Sr_2RuO_4) is a spin-triplet superconductor¹ of the Ruddlesden-Popper (RP) series with $n=1$. We have studied the electronic structure of single crystals of this system by density functional theory (DFT) calculations and soft x-ray emission and absorption measurements at the oxygen K edge (530 eV) and find that DFT calculations provide an excellent model to characterize the molecular orbitals corresponding to the inequivalent O sites in this perovskite compound. The linearly polarized radiation excites primarily O[1] (planar) sites at almost normal incidence and O[2] (apical) sites at grazing incidence. Our results suggest a larger level of hybridization between the Ru d and the O p states in the RuO_2 planes than between the Ru and apical O atoms, which also implies more localized bonding along the apical direction than the planar direction. This work was supported by DOE grant No. DE-FG02-05ER-46183. 1)Y. Maeno, et al, Nature 372, 532 (1994).

David Ederer
Tulane University

Date submitted: 30 Nov 2005

Electronic form version 1.4