Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Doping Evolution of Oxygen K-edge X-ray Absorption Spectra in Cuprate Superconductors[1] CHENG-CHIEN CHEN, Advanced Photon Source, Argonne National Laboratory, MICHAEL SENTEF, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, YVONNE KUNG, Department of Physics, Stanford University, CHUNJING JIA, Department of Applied Physics, Stanford University, RONNY THOMALE, Institute of Theoretical Physics, EPFL, BRIAN MORITZ, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, ARNO KAMPF, Center for Electronic Correlations and Magnetism, University of Augsburg, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — We study oxygen K-edge x-ray absorption spectroscopy (XAS) and investigate the validity of the Zhang-Rice Singlet (ZRS) picture in overdosed cuprate superconductors. Using large-scale exact diagonalization of the three-orbital Hubbard model, we observe the effect of strong correlations manifesting in a dynamical spectral weight transfer from the upper Hubbard band to the ZRS band. The quantitative agreement between theory and experiment highlights an additional spectral weight reshuffling due to core-hole interaction. Our results confirm the important correlated nature of the cuprates and elucidate the changing orbital character of the low-energy quasi-particles, but also demonstrate the continued relevance of the ZRS even in the overdosed region.

[1]This work is supported by the U.S. DOE under Contract No. DE-AC02-76SF00515.

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Date submitted: 23 Oct 2012 Electronic form version 1.4