

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Calculation of charge-transfer satellites in x-ray absorption spectroscopy of transition metal oxides¹ E. KLEVAK, University of Washington, J.J. KAS, U. Washington, J.J. REHR, University of Washington — Charge-transfer (CT) satellites in x-ray absorption spectroscopy (XAS) require treatments of correlation effects beyond the quasi-particle approximation. Here we present an approach for including CT effects in XAS that follows the model of Lee *et al.*² The approach is based on a three level system coupled to an itinerant state, with parameters obtained from either ab initio calculations or x-ray photoemission spectroscopy. The model yields an approximation to CT satellites in XAS in terms of a convolution of the quasi-particle spectrum with an energy-dependent spectral function that accounts for both localized CT excitations and solid state effects. The approach illustrates the crossover from the sudden to adiabatic approximations. Calculations for transition metal oxides, e.g. NiO and CoO, give reasonable agreement with XAS experiment. Finally, an extension of the present approach to CT satellites in resonant inelastic x-ray spectroscopy is also discussed.

¹Supported by DOE BES Grant DE-FG03-97ER45623.

²J.D. Lee, O. Gunnarsson and L. Hedin, Phys. Rev. B **60**, 8034 (1999)

E. Klevak
University of Washington

Date submitted: 15 Nov 2012

Electronic form version 1.4