

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Theory of K-edge resonant inelastic x-ray scattering and its application for $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$ ¹ T.F. SEMAN, New Jersey Institute of Technology, X. LIU, J.P. HILL, Brookhaven National Laboratory, M. VAN VEENENDAAL², Argonne National Laboratory, K.H. AHN, New Jersey Institute of Technology — We present a formula based on tight-binding approach for the calculation of K-edge resonant inelastic x-ray scattering spectrum for transition metal oxides, by extending the previous result [K. H. Ahn, A. J. Fedro, and M. van Veenendaal, Phys. Rev. B 79, 045103 (2009).] to include explicit momentum dependence and a basis with multiple core hole sites. We apply this formula to layered charge, orbital, and spin ordered manganites, $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$. The K-edge RIXS spectrum is found not periodic with respect to the actual reciprocal lattice, but approximately periodic with respect to the reciprocal lattice for the hypothetical unit cell with one core hole site. With experimental structure and reasonable tight-binding parameters, we obtain good agreement with experimental data, in particular, with regards to the large variation of the intensity with momentum. We find that the screening in $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$ is highly localized around the core hole site and demonstrate the potential of K-edge RIXS as a probe for the screening dynamics in materials.

¹Work supported by US.DOE Contr. DE-AC02-98CH10886 (X.L.,J.H.), US.DOE Award DE-FG02-03ER46097 (M.v.V.), CMCSN under Grants DE-FG02-08ER46540 & DE-SC0007091 (T.S.,K.A.,M.v.V.), Argonne XSD Visitor Prog.(K.A.), US.DOE Contr. DE-AC02-06CH11357 (X.L.,J.H).

²Northwestern Illinois University

Tsezar F. Seman
New Jersey Institute of Technology

Date submitted: 19 Nov 2012

Electronic form version 1.4