Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Final state lifetime effects in spectroscopic studies of iridium oxide J. MATTHIAS KAHK, DAVID J. PAYNE, Imperial College London — Understanding the complex and varied electronic and magnetic properties of late 3rd row transition metal oxides is a topic of significant current interest. The technique of Resonant Inelastic X-ray Scattering (RIXS) is particularly valuable in this field as it provides element- and orbital-specific information about the occupied and unoccupied electronic states. A major advantage of RIXS over techniques such as nonresonant XAS and XES is the sharpening of spectral features due to the absence of a core hole in both the initial and the final states. In typical simulations of RIXS spectra, final state lifetime effects are thus neglected, but this also precludes the possibility to account for the finite lifetime of the excited electron-hole pair created in the RIXS process. Starting from the well-known Kramers-Heisenberg equation, we have developed a new formalism for RIXS simulations which does allow for the inclusion of final state lifetime effects. Results are shown for the O K-edge RIXS of IrO_2, and the new formalism leads to a vast improvement in the agreement between theory and experiment. A similar approach also yields excellent agreement between theory and experiment for the nonresonant XAS and XES of IrO_2, as well as the valence band region of the IrO_2 HAXPES spectrum.

J. Matthias Kahk
Imperial College London

Date submitted: 23 Dec 2014 Electronic form version 1.4