Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Reciprocal space calculations of EELS and XAS spectra without the supercell[1] KEVIN JORISSEN, JOHN REHR, University of Washington — Traditionally, one has two ways of calculating *ab initio* x-ray and electron absorption spectra. Band structure calculations can treat periodic materials such as crystals, however, when a core hole is introduced and treated with a supercell approximation, unphysical interactions are often introduced. Real space calculations on the other hand, e.g. based on Green's function theory, can treat the core hole as an impurity, but have the disadvantage of finite cluster size effects. We present a hybrid method in which the perfect crystal is treated in reciprocal space, avoiding cluster size effects, and the inclusion of the core hole is done afterwards in real space, thus avoiding supercell effects. This strategy is implemented into the ab initio Green's function code FEFF8.6, which has recently been adapted for relativistic EELS-spectra. The method is illustrated, for example for the C K-edge of diamond.

[1]Supported by DOE Grant DE-FG02-97ER45623 (JJR) and facilitated by the DOE Computational Materials Science Network (CMSN). K. Jorissen acknowledges support by the Fonds voor Wetenschappelijk Onderzoek Vlaanderen.

Kevin Jorissen
University of Washington

Date submitted: 20 Nov 2006 Electronic form version 1.4