

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Many-Pole Self-Energy Model Corrections to Kohn-Sham Calculations of Excited State Spectra¹ J. J. KAS, M. PRANGE, J. J. REHR, H. M. LAWLER, University of Washington — Experimental x-ray spectra are systematically shifted and broadened with respect to conventional density functional theory calculations due to photoelectron self-energy effects. We have recently developed an efficient many-pole model of the GW self-energy based calculations of dielectric response using a real-space Green's function approach.² The model is applied *a posteriori* to Kohn-Sham calculations of excited state spectra using a convolution of the spectrum with an energy dependent Lorentzian. The method is found to be widely applicable over a broad range of energies, with little computational cost. Several illustrative examples are presented which show improved agreement between theoretical calculations and experiment for both optical and x-ray spectra.

¹Supported by NIH NCRB BTP grant RR-01209 (JK) and DOE Grant DE-FG02-97ER45623 (JJR and MP).

²J.J. Kas et al., Phys. Rev. B **76**, 195116 (2007).

Joshua Kas
University of Washington

Date submitted: 21 Nov 2008

Electronic form version 1.4