

Abstract Submitted  
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**Many-Pole Self-Energy Model Corrections to Kohn-Sham Calculations of Excited State Spectra**<sup>1</sup> 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.<sup>2</sup> 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.

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

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