Abstract Submitted
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Ab initio Calculations of X-ray Spectra: Comparison with Accurate Measurements[1] J. J. KAS, J. J. REHR, U. Washington, F. D. VILA — A number of advances in the theory of x-ray absorption (XAS) have been developed with the aim of achieving a parameter-free treatment of the key many-body effects.[2] These include a GW many-pole self-energy model, *ab initio* Debye-Waller factors, and an RPA screened core-hole. These developments have been implemented in the real-space multiple-scattering code FEFF9.0, and applied to calculations of x-ray absorption spectra and electron energy loss spectra as well as a variety of other core level spectroscopies. Calculations span a broad spectrum from the visible to x-ray energies. Results for a number of materials are compared with previous theories and with accurate experimental data.

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[2]J. J. Rehr et al., Comptes Rendus Physique, **10**, 548 (2009)

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