Theoretical investigation resolving discrepancies of atomic form factors and attenuation coefficients in the near-edge soft X-ray regime

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Reliable knowledge of the complex X-ray form factor and the photoelectric attenuation coefficient is required for crystallography, medical diagnosis, radiation safety and XAFS studies. Discrepancies between currently used theoretical approaches of 200% exist for numerous elements for X-ray energies from 1 keV to 3 keV [1,2]. This work addresses key discrepancies and derives theoretical results in near-edge soft X-ray regions.

DHF wavefunctions are employed and computational and convergence issues are of direct concern. Comparisons to simpler wavefunctions with additional relativistic corrections to the form factors are insightful.

The current result improves upon the theoretical uncertainty in these regions (to an estimated σ = 20% - 30%) and appears to reduce the error of this approach to less than one standard deviation. This work is a major new tabulation in J. Phys. Chem. Ref. Data [3].

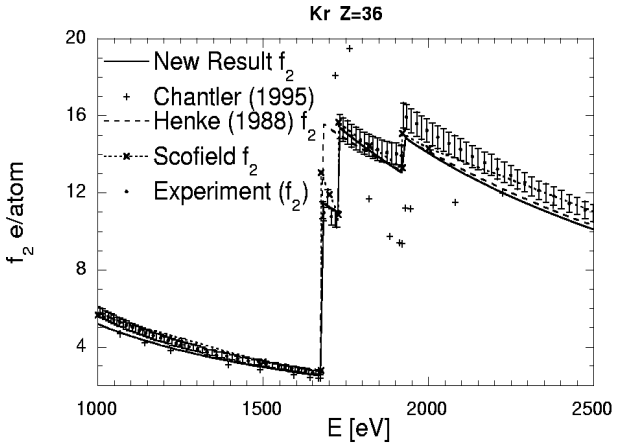

Figure 1: Plot illustrating the consistency of near-edge structure between experiment and that predicted by the new theoretical work, as opposed to earlier theory.

[1] Saloman, E.B., Hubbell, J.H., NBSIR 86-3431 (1986); Saloman E.B., Hubbell J.H., Scofield J.H., *At.Dat.Nucl.Dat.Tables* **38** (1988) 1-197.

[2] Chantler, C.T., *J. Phys. Chem. Ref. Data* **24** (1995) 71-643.

[3] Chantler, C.T., *J. Phys. Chem. Ref. Data* (2000) in press.