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Relativistic effects in EXAFS: overview and application to gold

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Current XAFS (X-ray Absorption Fine Structure) data-analysis is based on accurate multiple-scattering (MS) calculations, usually carried out solving the non-relativistic Schrödinger equation for complex effective optical muffin-tin potentials describing the scattering of the atoms. The introduction of relativistic effects in extended XAFS (EXAFS) multiple-scattering calculations has been described in several previous papers [1-4] and shown to be important for heavy atoms. However, few examples of applications and detailed studies of relativistic effects were given so far. In this work, we have performed a systematic investigation of relativistic corrections in systems of increasing atomic number, using a reliable simulation scheme based on the incorporation of a pseudo-Schrödinger equation [4-5] effectively replacing the Dirac relativistic form and incorporated in the GnXAS package for data-analysis [6,7]. Calculations have been put to a test in 12 different pure-element condensed-state systems, with the atomic number ranging from $Z = 10$ for crystalline Ne to $Z = 90$ for crystalline Th. The importance of accounting for relativistic effects has been highlighted for elements with $Z > 60$, as ones for which relativistic corrections for amplitudes of calculated XAFS MS signals exceed 10%. The impact of relativistic effects for calculated higher-order XAFS signal has been also evaluated for L3 and K edges, showing a slight increase of relativistic corrections for the L3 spectra. The present accuracy of XAFS simulations have been studied comparing the results obtained for structural refinements of the L3 edge of crystalline Au in a wide temperature range from 80 K to the melting point.

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