Coupled Cluster Strategies for Core Spectroscopies of Ground and Excited States

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Recent advances in synchrotron and free-electron laser sources have led to a renaissance in spectroscopic techniques in the x-ray region. More detailed experimental information can be obtained. New types of experiments are done and/or are envisaged. Theoretical calculations play an important role in the analysis and interpretation of experimental spectra. Advances in theory and data analysis that parallel the advances in experiment are required to retrieve quantitative chemical information.

Coupled cluster (response) approaches are undoubtedly among the most accurate ab initio techniques currently available for molecular properties and spectra, but their application to spectroscopies of core electrons is still somewhat limited. An overview of our work on the extension of Coupled Cluster Response Theory to compute Near-Edge Absorption Fine Structure spectra and photoelectron spectroscopy descriptors of both ground and excited states will be presented [1-10], including the results of a combined experimental and theoretical investigation of the transient NEXAFS Spectroscopy at the oxygen edge of thymine [10].

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