# Relativistic Coupled-Cluster Techniques for Calculation of X-ray Spectroscopy

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We present core-valance separated delta-coupled-cluster (CVS-ΔCC) methods with relativistic effects treated using the spin-free exact two-component theory in its one-electron variant (SFX2C-1e) for calculations of core-ionization energies. High-level relativistic (HLR) corrections beyond the SFX2C-1e, including the contributions from two-electron picture-change effects, spin-orbit coupling, the Breit term, and QED effects have also been considered and shown to play an important role for calculations of K-edge ionization energies of third-row elements. SFX2C-1e-CVS--ΔCCSD(T) calculations augmented with HLR corrections can provide accurate K-edge core ionization energies of second and third-row elements with deviation from experimental values less than 0.5 eV. Furthermore, we also present an edge-specific scheme for calculations of near edge X-ray absorption fine structure (NEXAFS) spectra using SFX2C-1e CVS-equation-of-motion coupled-cluster (CVS-EOM-CC) methods. Standard correlation-consistent basis sets for the atom where targeted core-excitation takes place are systematically augmented with diffuse functions to capture diffuse character of core excited Rydberg states. It has also been shown that triple excitations in CVS-EOM-CC methods not only are important for obtaining accurate absolute values for core excitation energies, but also make significant contributions to relative shifts between local and Rydberg core-excited states.