# SIMPLIFIED LR-TDDFT/ZORA APPROACH FOR GENERATING SPIN-ORBIT COUPLINGS FOR X-RAY ABSORPTION SPECTRA

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Transition metals represent a space of continual interest due to their complex electronic structure and the diverse range of possible ligands and oxidation states. Studies of transition metal complexes often rely on X-ray spectroscopies (usually at the L or M edges) and computational methods to explain spectral features and help design new experiments. Most computational approaches either account for relativistic effects at the scalar level, by omitting spin-orbit coupling terms, or completely neglect them sacrificing accuracy in favor of a lower computational cost. On the other hand, explicit ab-initio treatments of spin-orbit couplings are costly and labor intensive, restricting their applications to smaller atomic systems. In the present work, we propose a simplified approach based on linear-response time-dependent density functional theory (LR-TDDFT) and the relativistic two-component zeroth order regular approximation (ZORA) to generate spin-orbit couplings of closed-shell molecular systems. The proposed approach was validated by computing the L-edge absorption spectra of several first and second row transition metal complexes. The method reproduces experimental data with satisfactory accuracy at a fraction of the cost of exact two-component or fully relativistic methods.