# RESONANT INELASTIC X-RAY SCATTERING CALCULATIONS OF Ru COMPLEXES WITHIN A SIMPLIFIED TIME-DEPENDENT DENSITY FUNCTIONAL THEORY FRAMEWORK

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Resonant inelastic x-ray scattering (RIXS) provides valuable information on the electronic structure of molecules and materials that is not easily accessible by one-photon spectroscopies due to selection rule restrictions. With the continuing development in light source technologies, RIXS is rapidly becoming an important technique for the study of gas- and solution-phase molecular systems, and the need for reliable and inexpensive electronic structure methods to aid in the prediction and interpretation of complicated spectral features is becoming apparent. In this work, we present a simplified approach based on the linear-response time-dependent density functional theory (LR-TDDFT) formalism to simulate RIXS in 4d transition metal complexes without the need to solve the costly TDDFT quadratic-response equations. As an illustrative example, we simulate the 2p4d RIXS maps of three representative ruthenium complexes. The method is able to capture all experimental features in all three complexes with relative energies correct to within 0.6 eV, and at the cost of roughly two independent LR-TDDFT calculations.