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A TDDFT-based Method for the Calculation of Resonant Inelastic X-Ray Scattering in Condensed Phases

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Resonant Inelastic X-ray Scattering (RIXS) is a powerful photon-in/photon-out spectroscopic technique that provides unique, orbital-specific insights into electronic structure by probing excitations from a localized core orbital. Its accurate simulation for condensed-phase systems requires a method that simultaneously describes the local electronic structure of the absorbing atom and the extended environment while balancing computational cost with accuracy. We address this by presenting a new implementation of a RIXS module within the CP2K software package. Built upon CP2K's highly efficient linear-response TDDFT and XAS frameworks, this implementation presents the first generally available method for calculating RIXS spectra in both molecular and extended systems. We demonstrate the accuracy of our implementation on molecular systems and solutions, providing a robust approach for simulating RIXS spectra in complex environments.

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