Computational Techniques for Quantitative Prediction of X-Ray Absorption Spectroscopy

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X-ray spectroscopic techniques have found wide-spread applications in different areas of chemistry and biology. These techniques are often used to get information about the local electronic structure and solvent environment of an atom in large chemical systems. Computational techniques have played an essential role in analyzing and predicting X-ray spectroscopic signals for a wide-range of systems. Time-dependent density functional theory (TDDFT) is one of the most widely used techniques for X-ray spectroscopic calculations. However, this method does not always provide satisfactory quantitative and qualitative accuracy for the computation of X-ray spectroscopy of many open-shell systems like transition metal ions. In this talk, I am going to discuss some shortcomings of TDDFT and at the same time present other quantum chemical methods that can be useful in computing X-ray absorption spectroscopy.