

Wavefunction based approaches in X-ray spectroscopy

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With the aim to uniquely correlate spectroscopic properties to electronic structure and geometric properties of target materials, we employ in house developed wavefunction based methods in an effort to evaluate unique spectroscopic signatures of transition metal complexes and materials in both equilibrium and under operando conditions. This requires to use methods that do not belong in the standard arsenal of quantum chemistry. Over the last years we have developed and employed the restricted open shell configuration interaction singles methods (ROCIS and PNO-ROCIS) and their parameterized versions, (ROCIS/DFT and PNO-ROCIS/DFT)[1,2] to compute a large variety of XAS and valence to core resonance X-ray emission spectra (VtC-RXES) of classes of chemical systems ranging between molecules to ‘real-life’ molecular and solid systems [2,3]. Recently even more accurate computational protocols based on the complete active space configuration interaction in conjunction with N-electron valence second order perturbation theory (CASCI/NEVPT2)[4] as well as multireference configuration interaction (MRCI) and multireference equation of motion coupled cluster (MREOM-CC)[5] methods have been employed to compute challenging metal L-edge XAS spectra of medium sized molecules with high predictive accuracy. The talk will provide an overview of all the above methods and will explore their abilities in representative examples.

References

- [1] - M. Roemelt, D. Maganas, S. DeBeer and F. Neese, *J. Chem. Phys.*, **138**, 204101 (2013).
- [2] - D. Maganas, S. DeBeer, F. Neese, *J. Phys. Chem. A*, **122**, 1215 (2018).
- [3] - D. Maganas, S. DeBeer, F. Neese, *Inorg. Chem.* **56**, 11819 (2017).
- [4] - A. Chantzis, J. K. Kowalska, D. Maganas, S. DeBeer, F. Neese, *J. Chem. Theo. Comp.* **14**, 3686 (2018).
- [5] - D. Maganas, J. K. Kowalska, M. Nooijen, S. DeBeer, F. Neese, *J. Chem. Phys.* **150**, 104106 (2019).