Simulation of X-ray Absorption and X-ray Emission Spectroscopy

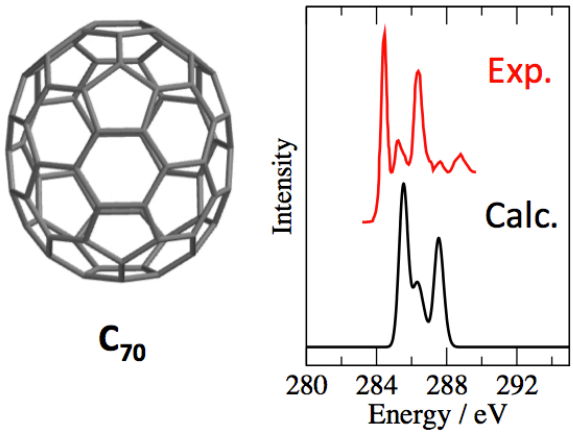
Nicholas A. Besley

School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

nick.besley@nottingham.ac.uk

In recent years, spectroscopy in the X-ray region has undergone tremendous advances due to the intensity and high resolution obtainable with synchrotron radiation. This has provided X-ray spectroscopy with a richness in structure that can match more traditional ultra-violet spectroscopy combined with the advantage that X-ray spectroscopy is element specific. Currently, the development of X-ray free-electron lasers that can deliver short femtosecond pulses of hard X-rays has opened up a new vista in time-resolved X-ray absorption measurements that hold the promise of resolving ultrafast chemical processes at an atomic level. Computational simulations of spectroscopy in the X-ray region play a critical role in the understanding and analysis of these experimental measurements.

In this talk an overview of recent developments in the application of time-dependent density functional theory (TDDFT) for the calculation of near-edge X-ray absorption fine structure (NEXAFS) spectroscopy and X-ray emission spectroscopy will be presented. It will be shown that the computational cost of TDDFT calculations of NEXAFS can be greatly reduced with negligible effect on the accuracy of the computed spectra, allowing much larger systems, such as C_{70}, to be studied.[1] The application of DFT and TDDFT with short-range corrected exchange-correlation functionals for the simulation of X-ray emission spectroscopy and resonant inelastic X-ray scattering will also be discussed.[2,3]



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References

[1] N.A. Besley, *J. Chem. Theory and Comput.*, **12**, 5018-5025 (2016)
[2] J. D. Wadey and N.A. Besley, *J. Chem. Theory and Comput.*, **10**, 4557-4564 (2014)
[3] I.P.E. Roper and N.A. Besley, *J. Chem. Phys.*, **144**, 114104 (2016)