Interference and Ionisation in Ultrafast X-ray Scattering

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Ultrafast x-ray scattering using x-ray free-electron lasers (XFELs) on free molecules in the gas phase provides a window onto dynamics induced by photon-absorption. Already, significant advances in resolving transient nuclear structural dynamics in excited molecules have been made [1-3]. Intriguingly, quantum interference effects are predicted to play a part in ultrafast x-ray scattering from electron dynamics [4-5] In this presentation, we investigate the role of ionisation in static and ultrafast non-resonant x-ray scattering using a molecular model system, which includes the ionisation continuum via an orthonormalised plane wave ansatz [6]. We examine the elastic and inelastic components of the scattering signal, as well as the coherent mixed scattering that arises from electron dynamics [7-8]. We find that ionisation contributes significantly to the inelastic and coherent mixed components, especially at intermediate and high momentum transfer. We conclude with recommendations regarding the accuracy of theoretically predicted scattering signals and a general outlook on potential experiments sensitive to electron dynamics.

References

[1] Minitti *et al.* Phys. Rev. Lett. **114** 255501 (2015)
[2] Stankus *et al.* Nature Chem. **11** 716 (2019)
[3] Ruddock *et al.* Science Adv. **5** eaax6625 (2019)
[4] Simmermacher *et al.* Phys. Rev. Lett. **122** 073003 (2019)
[5] Simmermacher *et al.* J. Chem. Phys. **151** 174302 (2019)
[6] Ziems *et al.* (under review)
[7] Moreno Carrascosa *et al.* J. Chem. Theory Comp. **15** 2836 (2019)
[8] Zotev *et al*. J. Chem. Theory Comp. **16** 2594 (2020)