European XFEL Theory Seminar

Thursday 13th December 2018, 17:00
Campus Schenefeld, XHQ, room E1.096

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Ultrafast X-ray scattering: chemical dynamics and beyond

Scattering experiments that use X-ray Free-Electron Lasers (XFELs) provide new and exciting opportunities for the study of ultrafast photochemical and photophysical processes[1,2]. We present simulations of nonresonant ultrafast X-ray scattering from a molecular wavepacket and examine the components that contribute to the total scattering signal. The simulations demonstrate how the elastic component, which can be used to determine the spatio-temporal structural dynamics of the molecule, also carries an imprint of the electronic structure, and that interferences play an important role in the scattering[3]. As part of the talk, we will discuss recent experiments on molecules in the gas-phase, with a particular focus on the intersection of theory, simulations, and experiments [4,5,6].

[1] M. P. Minitti *et al.* Phys. Rev. Lett. **114** 255501 (2015)
[2] B. Stankus *et al.* Faraday Disc. **194** 525 (2016)
[3] G. Dixit, O. Vendrell, R. Santra PNAS **109** 11636 (2012)
[4] A. Kirrander *et al.*, J. Chem. Theory Comput. **12**, 957 (2016)
[5] A. Kirrander, P. M. Weber Applied Science **7**, 534 (2017)
[6] H. Yong *et al.* J. Phys. Chem. Lett. **9**, 6556 (2018)

Host: Evgeny Gorelov