

SEMINAIRE ISMO

Adam Kirrander

School of Chemistry, University of Edinburgh, United Kingdom

Ultrafast X-ray scattering: chemical dynamics and beyond

Ultrafast scattering using X-ray Free-Electron Lasers (XFELs) is an exciting development in AMO physics and chemical reaction dynamics. The elastic component of the scattering provides a direct probe of structural dynamics, as demonstrated in recent experiments (see Fig. 1a). The experiments are supported by ab initio electronic structure calculations and quantum molecular dynamics simulations.

From a theoretical point of view, the standard expressions for X-ray scattering are modified by the quantum superposition inherent in ultrafast experiments. I will demonstrate how the wavepacket limits the spatial resolution attainable in diffraction experiments (see Fig. 1b), and discuss how interference effects might make it possible to characterize electronic transitions during nonadiabatic dynamics.

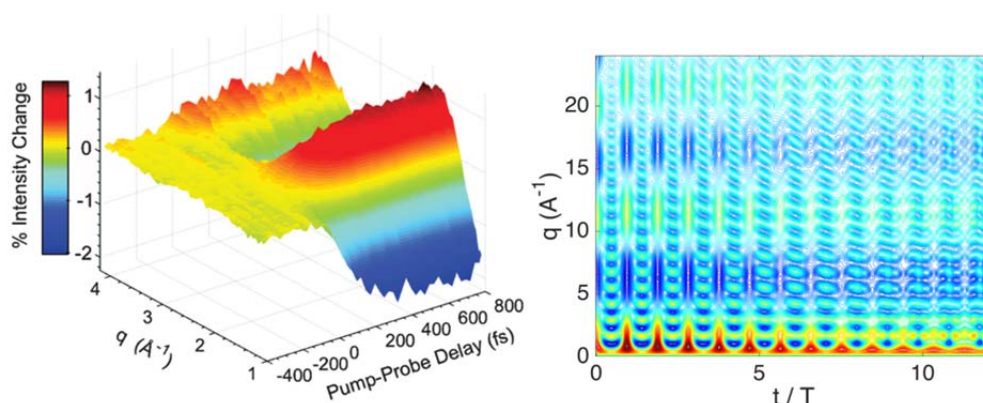


Fig. 1. (a) Scattering from 1,3-cyclohexadiene

(b) Scattering from a dispersing wavepacket in D_2 molecule

Mardi 29 mai 2018 à 11 h
Amphithéâtre du bât 520 (3^{ème} étage)
Université Paris-Sud - 91405 ORSAY Cedex