Ultrafast X-Ray Scattering: Chemical Dynamics and Beyond

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Ultrafast scattering using x-ray free-electron lasers such as the LCLS in California is an exciting new development in the study of chemical reaction dynamics [1]. The elastic component of the scattering provides a direct probe of structural dynamics of a molecule as it reacts, as demonstrated in recent experiments [2,3] (Fig. 1a). The experiments are supported by *ab initio* electronic structure calculations and quantum molecular dynamics simulations.

From a theoretical point of view, one must be careful how the standard expressions for x-ray scattering are modified when scattering of coherent x-rays from a quantum superposition is considered [4]. I will demonstrate how the wavepacket limits the spatial resolution attainable in diffraction experiments [5] (see Fig. 1b) and discuss how interference effects might make it possible to characterize electronic coherences during the dynamics.

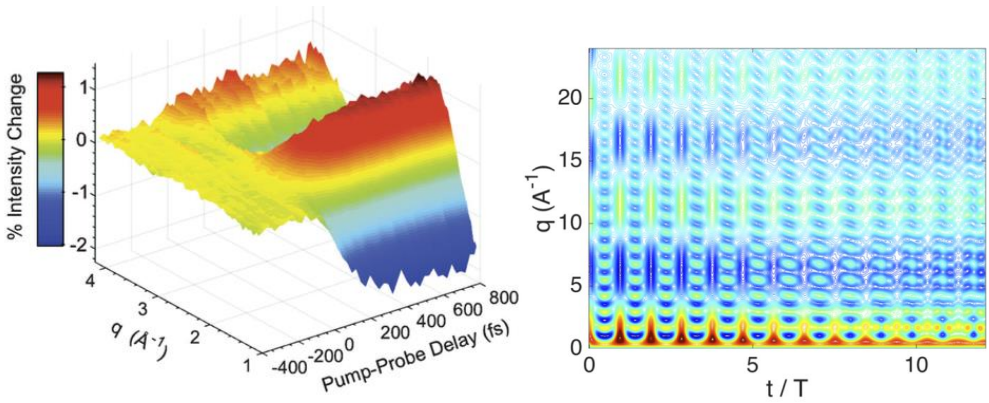

Fig. 1. (a) Scattering from 1,3-cyclohexadiene [1]; (b) Scattering from a dispersing wavepacket in D_2 molecule [5].

References

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