Imaging Ultrafast Electronic Motion by Time-Resolved X-ray Scattering

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Imaging the motion of electrons during physical, chemical and biological processes in real-space and in real-time is of interest as it can provide important insights into the mechanisms involved. Although scattering of ultrashort x-ray pulses from electronic wave packets is a promising approach for realizing this goal, but there are still some questions about the feasibility of achieving such imaging. I will discuss the problem of using ultrafast x-rays for imaging the time evolution of nonstationary electronic systems. The practical importance of electronically elastic x-ray scattering from materials derives from the fact that for an electronically stationary sample, the x-ray scattering pattern is related to the electron density distribution in the sample. With the advent of ultrafast x-ray sources, it is natural to envision viewing the motion of electrons using time-resolved x-ray scattering. It is tempting to assume that the x-ray scattering pattern that would be observed can be understood through the x-ray scattering theory for electronically stationary targets. This approach would suggest that time-resolved x-ray scattering with a sufficiently short x-ray pulse probes the instantaneous electron density in the sample. In this talk, I will show that, in general, this expectation is not only quantitatively, but also qualitatively incorrect [1-3]. I will close by proposing a possible way to image the instantaneous electron density of electronic wave packets via ultrafast x-ray phase contrast imaging [4]. I will show that inelastic scattering processes, which plague ultrafast scattering in the far-field regime, do not contribute in ultrafast x-ray phase contrast imaging as a consequence of an interference effect. This approach also provides the Laplacian of the instantaneous electron density, which can be used to garner details of the internal structures of the wave packet. This may be useful for understanding complex bonding and topology of charge distributions in complex systems.

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[2] G. Dixit, and R. Santra, **J. Chem. Phys**. **138**, 134311 (2013).

[3] G. Dixit, J. M. Slowik and R. Santra, (to be published).

[4] G. Dixit, J. M. Slowik and R. Santra, **Phys. Rev. Lett. 110**, 137403 (2013).