CFEL SCIENCE

SEMINAR

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CFEL – Building 99, seminar room I+II (ground floor)

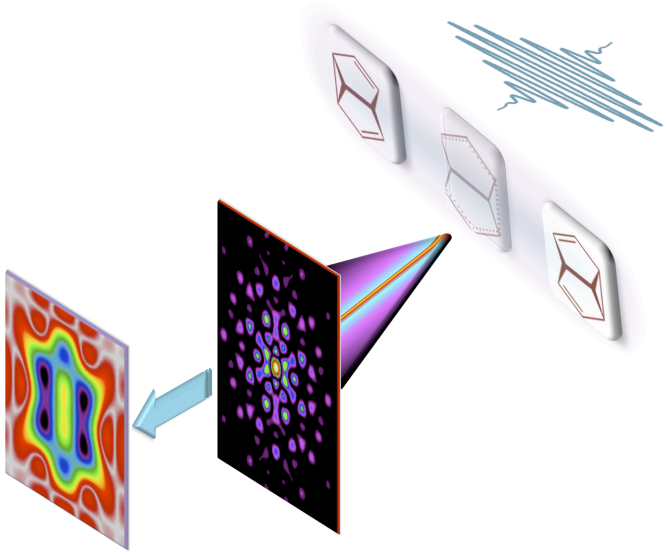
Gopal Dixit

Max-Born Institute, Berlin, Germany

X-ray imaging of chemically active valence electrons during a chemical reaction

Time-resolved imaging of chemically active valence electron densities is a long-sought goal, as these electrons dictate the course of chemical reactions. The ultrashort x-ray pulses from XFELs promise to provide stroboscopic snapshots of chemical processes by extending static diffraction techniques into the domain of ultrafast electronic processes. However, x-ray diffraction from active valence electrons is very weak in comparison with that from inactive valence and core electrons. The active valence electron density contributes only a very small fraction to the total diffraction pattern, which makes use of x-ray diffraction for time-resolved imaging of changes in chemically relevant parts of the valence electron density during complex chemical reactions extremely challenging.

In our recent work we demonstrate a way to resolve this challenge. In this work, we theoretically demonstrate a robust and effective method to extract the contributions of chemically active valence electrons from the total x-ray diffraction by a single molecule [1]. By combining the standard analysis of the full x-ray diffraction pattern with an additional analysis of the part of the diffraction pattern, which is limited to relatively small momentum transfer, one nearly effortlessly brings to the fore the motion of chemically active valence electrons. Our work not only showed how to film chemically active valence electrons with x-rays, it has also provided an experimental access to the long-standing problem: Are the new bonds made at the same time as old bonds are broken (synchronous), or is there a time-delay between these two processes (asynchronous)? The degenerate Cope rearrangement of semibullvalene, a pericylic reaction, is chosen to demonstrate our proposed method.



[1] Timm Bredtmann, Misha Ivanov and Gopal Dixit, "X-ray imaging of chemically active valence electrons during a pericyclic reaction" *Nature Communications* **5**, 5589 (2014).

Host: Terry Mullins / CFEL Molecular Physics Seminar