European XFEL Science Seminar

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Zoom Meeting

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Mapping Atomic Motions with Ultrabright Electrons: Fundamental Space-Time Limits to Imaging Chemistry

One of the long sought objectives in science has been to watch atomic motions on the primary timescales governing structural transitions. From a chemistry perspective, this capability would give a direct observation of reaction forces and probe the central unifying concept of transition states that links chemistry to biology. To achieve this objective, there are not only extraordinary requirements for simultaneous spatial-temporal resolution but equally important, due to sample limitations, also one on source brightness. With the development of ultrabright electrons capable of literally lighting up atomic motions, this experiment has been realized (Siwick et al Science 2003) and efforts accelerated with the onset of XFELs (Miller, Science 2014). A number of different chemical reactions will be discussed from electrocyclization with conserved stereochemistry, intermolecular electron transfer for organic systems, metal to metal electron transfer, to the direct observation of a bimolecular collision and bond formation in condensed phase for the classic I_3^- system, in a process analogous to a molecular Newton's cradle. These studies have discovered that these high dimensional problems, order 3N (N number of atoms in the reaction volume) representing the number of degrees of freedom in the system, distilled down to atomic projections along a few principle reaction coordinates. The specific details depend on the spatial resolution to these motions, for which <.01 Å changes in atomic position (less than the background thermal motion) has now been achieved on the 100 fs timescale. Without any detailed analysis, the key large-amplitude modes can be identified by eye from the molecular movies. This reduction in dimensionality appears to be general, arising from the very strong anharmonicity of the many body potential in the barrier crossing region. We now are beginning to see the underlying physics for the generalized reaction mechanisms that have been empirically discovered over time. The "magic of chemistry" is this enormous reduction in dimensionality in the barrier crossing region that ultimately makes chemical concepts transferrable. How far can this reductionist view be extended with respect to complexity? This direct observation of the key reaction modes and reduction principle at play is also providing new insight into how chemistry scaled up to the level of biological functions.This talk will also address the prospect of imaging single molecule trajectories and possibility of quantum tomography to go beyond the classical picture of structural dynamics to retrieve nuclear and electron probability distributions.

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