

"Making the Molecular Movie" Quest for the Structure-Function Correlation in Biology

Femtosecond Electron Diffraction harbours great potential for providing atomic resolution to structural changes as they occur, essentially watching atoms move in real time --- directly observe transition states. This experiment has been referred to as "making the molecular movie" and has been previously discussed in the context of a gedanken experiment.

With the recent development of femtosecond electron pulses with sufficient number density to execute nearly single shot structure determinations, this experiment has been finally realized. A new concept in electron pulse generation was developed based on a solution to the N-body electron propagation problem involving up to 10,000 interacting electrons that has led to a new generation of extremely bright electron pulsed sources that minimizes space charge broadening effects.

Previously thought intractable problems of determining $t=0$ and fully characterizing electron pulses on the femtosecond time scale have now been solved through the use of the laser ponderomotive potential to provide a time dependent scattering source. Synchronization of electron probe and laser excitation pulses is now possible with an accuracy of 10 femtoseconds to follow even the fastest nuclear motions. The camera for the "molecular movie" is now in hand

Atomic level views of the simplest possible structural transition, melting, have been obtained for a number of systems involving both thermal and purely electronically driven atomic displacements. Optical manipulation of charge distributions and effects on interatomic forces/bonding can be directly observed. These new developments will be discussed in the context of developing the necessary technology to directly observe the structure-function correlation in biomolecules – the fundamental molecular basis of biological systems.