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Ultrafast Dynamical Study Using Time-resolved Laue Diffraction

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Electron transfer reactions are fundamental processes in chemistry and also in biology [1-3]. Light harvesting complexes are functional centers in plants where sunlight is converted into chemical energy. In this, optical excitation in a chromophore unit leads to the transfer of electrons within the system. However, due to the complexity of the biological photo-reaction centre, recent spectroscopic efforts have concentrated on a smaller chemical model which share characteristic with their biological counter parts. A promising model is the so-called D-A (donor-acceptor) systems, which are chemically synthetic molecules with electron transfer capabilities. The electrical conductivity is a function of the optical state of the system. An optically switching diode is an interesting application of donor-acceptor molecules. We aimed to determine photo-induced structural changes in Pyrene-N,N-dimethylaniline (PyDMA). Static structures for many molecules are available at high resolution but the mechanism by which these molecules function and the structures of intermediate states often remain elusive. Knowledge of the geometry of molecular excited states at atomic resolution is crucial for a full understanding of photo-induced chemical processes. Time-resolved X-ray diffraction (TR-XRD) using polychromatic synchrotron radiation allows a detailed study of the time evolution of structural intermediates and short living states of chemical systems at wide range of time-scales, drawing a complete picture of the photo-induced charge transfer process. Investigation of photo-excitation processes in molecular single crystals, where the initial photo-excitation processes occur on extremely short time-scales (femto-/picosecond time domain) and have been in the focus of scientific investigations due to their possible applications, e.g. as optical switches.

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