Photoinduced structural dynamics of solvated molecules with X-ray scattering

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The tracking of atomic motions in real time upon photoexcitation of molecules in solution is achieved through time resolved X-ray scattering at X-ray Free Electron Lasers. Femtosecond X-ray pulses allow the direct observation of the photoinduced vibrational and rotational coherences of solvated transition metal complexes, together with the changes of the solvation shells in response to the rearrangements of the atomic and electronic structure of the solute upon the photoexcitation. We investigate the femtosecond photoinduced solute and solvent dynamics of a Co complex [1] and a di-Platinum complex in water with time-resolved X-ray scattering. We observe vibrational modes of the solute both in the ground and in the excited state potentials and rotational dephasing following the photoselection. We furthermore directly observe solvation effects [2], the impulsive response of the water molecules to the electric field of the laser pulse [1], and the transfer of excess energy from the solute to the solvent, from which the energetics of the excited states can be derived [3].

References:

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