Molecular dynamics studied by picosecond X-ray diffraction

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Abstract: The excited-state structure of small molecules in solution has been studied by combining ultrafast laser techniques with x-ray diffraction. The experiments are done using the pump and probe method: short laser pulses (1 ps) excite a subset of molecules in the sample and delayed x-ray pulses (100 ps) record the structure at a given delay. The diffraction patterns are recorded on a CCD detector in pairs *with* and *without* excitation. The change in the intensity $\delta S(q, t)$ is then Fourier transformed to $\delta S[r, t]$, the real-space image of the excited system. There are two contributions to $\delta S[r, t]$: the *change* in intramolecular structure of the solute in its cage and the *change* in intermolecular structure in the bulk liquid. We have studied these phenomena for some simple photo reactions in liquids: the dissociation and recombination of I_2[1,2], HgI_2, $C_2H_4I_2$ and Br_2 in polar and non-polar liquids. The experimental data will be compared to Molecular Dynamics simulations and we will discuss methods to separate the two contributions.
Finally we will discuss our myoglobin project, specifically the migration of CO in native myoglobin and in the mutant L29F. In both cases the difference maps show how CO moves away from the binding site in jumps between cavities in the protein [3].

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[2] Ultrafast X-ray Diffraction of Transient Structures in Solution", H. Ihee, M. Lorenc, T. K. Kim, Q. Y. Kong, M. Cammarata, J. H. Lee, S. Bratos, M. Wulff,
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[3] "Watching a Protein as it Functions: 150 ps Time-resolved Structures of a Myoglobin Mutant at 1.7 Å Resolution"
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