Ultrafast structural characterization of solvation dynamics with X-ray Solution Scattering

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The complex phenomenon of solvation, which is the local structural (re-) arrangements of the solvent molecules around a given solute species, is involved in many chemical reactions of biological and technological importance. The average local structure of in particular water around a wide range of solute species has been studied for many years with a multitude of methods[1,2] . However, due to the ultrafast time scales involved, the actual structural dynamics which take place during a chemical reaction have been much harder to study and comparatively little is known about the solvation structure(s) of transient chemical species. This presentation seeks to discuss a few cases where such dynamics are of importance for the outcome of (photo) chemical reactions[3,4] and to highlight how the high structural sensitivity and ultrafast temporal resolution of 4th generation X-ray sources can be utilized to shed light on these phenomena. In particular, the talk will focus on some very recent results obtained for the structural characterization of the ultrafast solvation dynamics following photo-abstraction of electrons from the I^- and Br^- halides in aqueous solution and on how detailed analysis based on Molecular Dynamics modelling can provide insights into the molecular-level interactions between solute and solvent molecules.

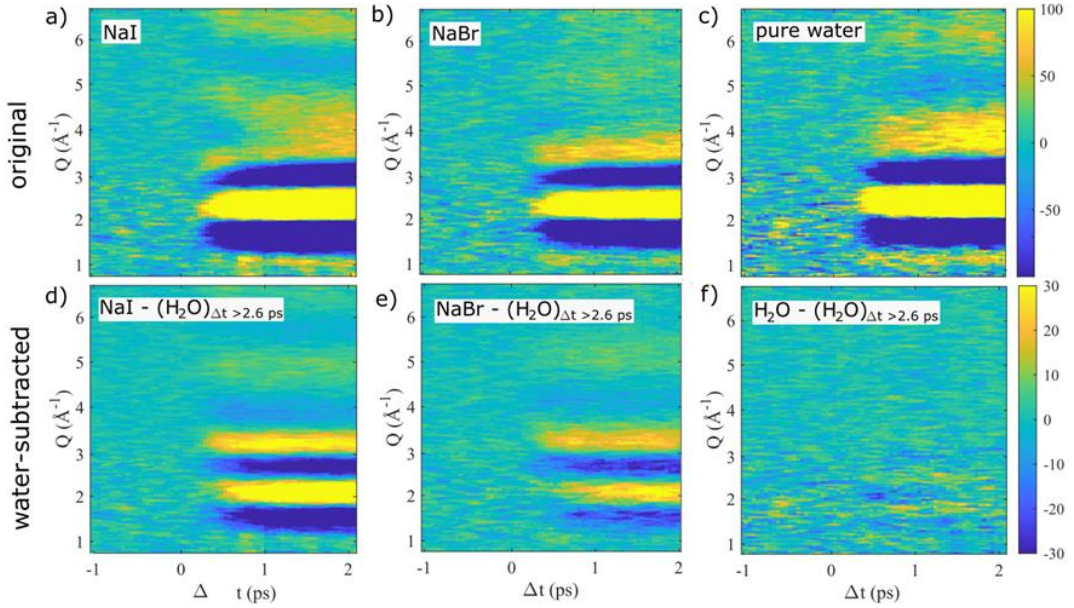

Figure 1: Top: Time-Resolved X-ray difference scattering signals following 200 nm excitation of solutions of NaI, NaBr and neat water. Bottom: Same difference signals, following subtraction of the contribution from heating of the aqueous solvent. Clear X-ray scattering signatures from the ultrafast changes in solvation structure can be seen and analyzed in detail.

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References

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