Contribution ID: **73** Type: **Keynote**

Opportunities in Non-equilibrium (Bio)chemistry via THz-driven Water Dynamics

Wednesday, 7 September 2022 11:30 (30 minutes)

Liquid water is the single most important medium in which highly consequential chemical and biological processes take place. Water is often equivocally regarded as a passive medium. Ranging from an isolated molecule to small clusters and up to bulk, water shows unique and ubiquitous behavior at different temperatures and environments. The main reason is the presence of a strong H-bond network[1], which is why water provides a very dynamic environment to solutes.

The H-bond network plays a crucial role in the vast majority of solvation chemical reactions, such as femtosecond guest-host interactions, folding processes in biomolecules, and non-equilibrium chemical kinetics, which are not light-triggered reactions but kinetically activated. The combination of ultrafast strong-field THz[2] and X-ray sources[3] forges a unique opportunity to drive and visualize water molecular dynamics for in-solvation (bio)chemical reactions to be understood and controlled. First, before its thermalization, investigating the non-equilibrium, femtosecond to picosecond time evolution of the structure of water clusters under strong-field THz radiation renders H-bond network disruptions resembling supercritical-like water structure that may play a crucial chemical role via interactions with the first few hydration shells and beyond. Second, the H-bond network relaxation and thermalization at longer delays (»100s of picosecond) will also yield tunable temperature jumps (T-jumps) from a fraction to hundreds of Kelvin.

In this talk, we will first review recent advancements in THz-driven non-equilibrium in-solution biochemistry. We will also discuss how understanding the ultrafast non-equilibrium and thermalization processes of water under THz excitation could unlock a vast ensemble of physical and biological quantum chemistry in highly disrupted hydration shells that are not possible to study today. Last, we will summarize the scientific and technological challenges ahead to fully capitalize on this generalized framework.

References:
[1] Aquino, J. Phys. Chem. A 106, 1862 (2002)
[2] Carbajo, Optics letters 40.24 (2015): 5762-5765; Ravi, Optics express 22.17 (2014): 20239-20251
[3] Amann, Nature photonics 6.10 (2012): 693-698; Schoenlein, Philosophical Transactions of the Royal Society A 377.2145 (2019): 20180384; Arnold, The Journal of Chemical Physics 150.4 (2019): 044505

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No

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Session Classification: XFEL II