CFEL SCIENCE

SEMINAR

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Zoom virtual meeting https://desy.zoom.us/j/99570520017

(Meeting-ID: 995 7052 0017, Password: 911851)

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Ionization and fragmentation of bio-relevant molecules: the influence of neighbours

Ionizing radiation penetrating biological tissue produces large numbers of secondary electrons which effectively induce damages in bio-molecules. Here using a multi-particle coincidence technique (reaction microscope) we investigate how the electron-impact induced fragmentation processes of molecular monomers are modified by the environment in the condensed phase. A model system is tetrahydrofuran (THF, C_4H_8O) a five membered ring that is often regarded as the simplest surrogate for the sugar deoxyribose in the DNA backbone. THF is capable of one hydrogen-bonding link to water and forms reasonable simple THF-water dimers electronic structure calculations are feasible.

In contrast to the expectation that a water environment quenches THF fragmentation by dissipating energy we find that water can catalyze THF ring-break reactions. Compared to the monomer the reaction barrier for the ring-break reaction is reduced in hydrated THF such that ionization of the HOMO is sufficient to break the molecular ring. Furthermore, we were able to experimentally identify intermolecular Coulombic decay (ICD) in THF-H_2O dimers. In this energy transfer process an initial electron-vacancy in water decays by ionizing the neighboring THF molecule. Recent experiments also show evidence of ICD among two organic molecules such that it appears to be a general and relevant damage mechanism in irradiated organic tissue.

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar