CFEL SCIENCE

SEMINAR

11th February 2026 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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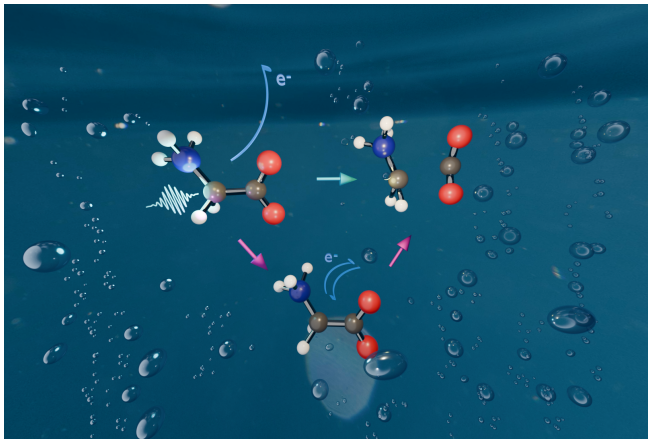
Ultrafast radiation chemistry of glycine in aqueous solution



Amino acids are fundamental building blocks of life, and their behavior in aqueous environments is central to many biological processes. Despite extensive research, key aspects of their radiation chemistry in water remain unresolved. Understanding their ionization-induced dynamics is therefore essential, with important implications in space travel and cancer therapy.

I present a computational study of ionization-induced dynamics of glycine in aqueous solution using the fewest-switches-surface hopping approach. We investigate ionization events occurring in different molecular orbitals of glycine as well as in the water molecules of its solvation shell.

Our results reveal three main findings. First, upon ionization, glycine undergoes rapid fragmentation on its Cα–C bond. We identify the main mechanisms leading to the dissociation products: CO_2 and the methylamine ($+H_3NH_2C\cdot$) radical. Second, ionization of deeper-lying orbitals triggers electronic relaxation to the ground state prior to fragmentation. Finally, we identify redox reactions between glycine and water. Overall, these results provide new insight into the radiation chemistry of the system.

Host: Robin Santra – CFEL-DESY Theory Division