# First principles simulations of biological matter subjected to ionizing radiations

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The transient collision of high-energy-transfer particles with matter results in ionization or excitation of its constituent molecules. Huge amounts of energy are deposited locally, typically several tens of eV, with copious emission of low energy electrons[1]. These early physical events produce a myriad of reactive radical species that are at the source of cascades of chemical processes spanning several spatial and temporal scales. The physical chemistry of these ultrafast processes is not well understood at the present time. First principle simulations would bring valuable insights on the mechanisms involved at the molecular scale and help interpret ultrafast experiments (e.g. attosecond spectroscopy or pulse radiolysis).

We have embarked on a long-term research program aiming at devising innovative approaches to simulate energy deposition and ultrafast reactivity within complex matter (e.g. biological matter). Our approaches are based on Density Functional Theory (ADFT) Real-Time Time Dependent ADFT and Molecular Dynamics (MD) simulations[2,3]. A hybrid scheme coupling these approaches to polarizable force fields have been devised[4]. Theses methodologies have been implemented in deMon2k. They allow simulations of collisions of molecules with fast ions or ionization by ionizing photons, ultrafast charge migration, energy relaxation/dissipation on the attosecond time scale (cf. Figure) for systems comprised of up to 1,000 atoms[5]. MD further gives access to chemical reactivity taking place in the first picosecond after irradiation[6].

I will introduce the methodologies and applications to various questions of current high interest in radiation chemistry.

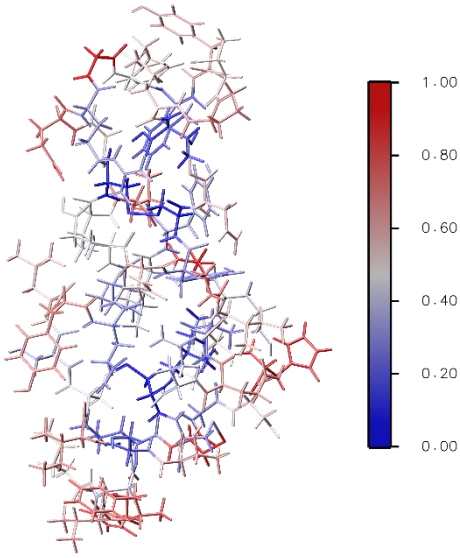


Figure 1: our RT-TD-ADFT methodology permits to investigate XUV irradiation of large biological molecules and revearl key insights on the ionization mechanism.

References:

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