Ab initio atomistic simulations of the physical and physico-chemical stages of ionizing irradiation of matter

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Molecular-scale ab initio simulations of ionizing irradiation of matter remain a major challenge due to the complexity of the physical and chemical processes to be captured[1]. Yet such simulations would be extremely valuable for understanding in detail the mechanisms of radiation-induced degradation, for example of complex biomolecules.

At ICP Orsay, we are developing original approaches based on the formalism of time-dependent density functional theory to describe the physical and physico-chemical stages of ionizing irradiation. These developments, carried out as part of the deMon2k program, are now available to the community on the Zenodo platform (https://zenodo.org/records/10528681).

In this presentation, I'll review the current status of our developments[2], before moving on to some examples of recent applications. These include the interpretation of attosecond pump-probe spectroscopy experiments on proteins - to the best of our knowledge the only one of its kind in the world to date - and picosecond pulsed radiolysis experiments[3].

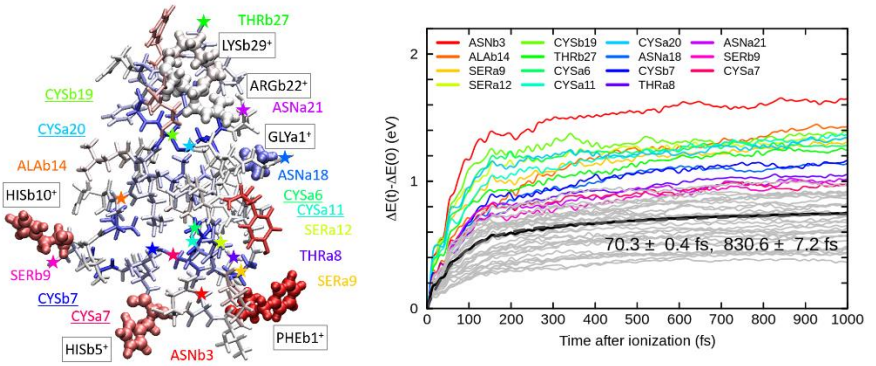

Figure 1: XUV ionization induces relaxation of a protein.

[1] Omar K A, Hasnaoui K and de la Lande A 2021 First-Principles Simulations of Biological Molecules Subjected to Ionizing Radiation *Annu. Rev. Phys. Chem.* **72** 445–65

[2] Omar K A, Korsaye F A, Tandiana R, Tolu D, Deviers J, Wu X, Parise A, Alvarez-Ibarra A, Moncada F, Pedroza-Montero J N, Mejía-Rodriguez D, Van-Oanh N-T, Cailliez F, Clavaguéra C, Hasnaoui K and de la Lande A 2023 Current status of deMon2k for the investigation of the early stages of matter irradiation by time-dependent DFT approaches *The European Physical Journal Special Topics* **232** 2167–93

[3] de la Lande A, Denisov S and Mostafavi M 2021 The mystery of sub-picosecond charge transfer following irradiation of hydrated uridine monophosphate *Phys. Chem. Chem. Phys.* **23** 21148–62