

Atomistic Modelling of Hadron Radiation Damage to DNA: from Stopping Powers to Reaction Kinetics

Stephan P. A. Sauer

Department of Chemistry, University of Copenhagen, Denmark

Abstract: Hadron therapy, i.e. the use of protons and C^{6+} ion beams instead of photon beams in radiation therapy, is an upcoming new way of treating cancer. Compared to standard radiation therapy it offers the advantage of reduced damage to the surrounding tissues. Over the recent years, we have been trying to cast light on some of the molecular processes which will finally lead to the strand breaks in DNA.

We have on one hand focused on the initial, physical interaction of the ion beam with different kind of molecules in a cell. This involves an energy transfer to the target molecule leading to its ionization or fragmentation and a slowing down of the ion beam projectiles. The key property in this process is the stopping power of the target, which in the Bethe theory [1] is directly related to the mean excitation energy of the target. The latter can accurately be calculated from the poles and residues of the linear response function of the electric dipole moment operator. In my talk I will illustrate this for several classes of molecules [2-6].

One of the most important target molecules is water, whose fragmentation leads to the formation of OH-radicals. In a second line of research we have studied possible reactions of the OH-radical with DNA. In my talk I will present first results of our atomistic modelling of the reaction of OH-radicals with the five nucleobases and discuss the importance of several aspects of the ab initio calculations of these reactions [7-9].

References:

[1] H. Bethe, Ann. Phys. 397, 325-400 (1930).

[2] S. P. A. Sauer, J. Oddershede, J. R. Sabin, J. Phys. Chem. A 110, 8811-8817 (2006)

[3] S. Bruun-Ghalbia, S. P. A. Sauer, J. Oddershede, J. Phys. Chem. B 144, 633-637 (2010)

[4] S. Bruun-Ghalbia, S. P. A. Sauer, J. Oddershede, J. R. Sabin, Eur. Phys. J. D 60, 71-76 (2010)

[5] S. P. A. Sauer, J. Oddershede, J. R. Sabin, J. Phys. Chem. C 114, 20335-20341 (2010)

[6] S. P. A. Sauer, J. Oddershede, J. R. Sabin, Adv. Quantum Chem. 62, 215-242 (2011)

[7] B. O. Milhøj, S. P. A. Sauer, J. Phys. Chem. A 119, 6516-6527 (2015)

[8] B. O. Milhøj, S. P. A. Sauer, Chem. Eur. J. 21, 17786–17799 (2015)

[9] B. O. Milhøj, S. P. A. Sauer, ChemPhysChem 17, 3086–3095 (2016)