Ionization and fragmentation of isolated biomolecules and their clusters

Jos Postma, Sadia Bari, Ronnie Hoekstra, Thomas Schlathölter

KVI Atomic Physics, University of Groningen, The Netherlands

tschlat@kvi.nl

The interaction of keV protons and heavy ions with building blocks of DNA is of particular biological relevance in view of the increasing number of facilities employing MeV proton and heavy ion irradiation for tumor treatment. When the ions traverse tissue and are decelerated to sub-MeV energies, the so-called Bragg-peak is reached where the induced damage is highest due to maximum linear energy transfer (LET) and relative biological effectiveness (RBE) at these energies. The volume selectivity given by the existence of such a well-localized Bragg-peak region renders proton therapy such a promising tool for cancer treatment [1]. Biological consequences of irradiation with energetic protons and heavy ions from galactic cosmic rays and solar particle events are also a limiting factor for human space exploration.

Radiation damage in living cells always involves the condensed phase where the affected molecules are surrounded by a medium. Therefore, ion irradiation studies on nucleobases in the solid phase [2] and on DNA deposited on substrates [3] have been performed. Such studies are however hampered by the great complexity of the systems under study.

A natural solution to avoid these difficulties is the investigation of smaller systems. We investigate the response of isolated DNA building blocks, and their clusters upon keV singly and multiply charged ion impact using high-resolution coincidence time-of-flight mass spectrometry. Kinetic energies of nucleobase and amino-acid fragments exceeding several 10 eV are observed which have the potential to induce subsequent damage in a biological environment [4,5]. Deoxyribose molecules from the DNA backbone are found to be most sensitive to keV ion impact and are subject to statistical fragmentation[6].

To bridge the gap between the biologically relevant condensed phase regime of and experiments on isolated molecules, we investigate systems still allowing intermolecular interactions. Our recent studies on clusters of nucleobases e.g. reveal that intermolecular hydrogen bonds strongly affect the fragmentation dynamics of the DNA building blocks [7].

Currently we are performing irradiation experiments on more complex biomolecular targets, produced by means of electrospray ionization. It is the goal of these studies to investigate well defined DNA oligomers surrounded by a tunable number of water molecules which can be considered good model systems of DNA and its closest environment.

[1] G. Kraft, Nucl. Instrum. Meth. B **454** (2000) 1
[2] Z. Deng, I. Bald, E. Illenberger and M. A. Huels, PRL **95** (2005) 153201
[3] S. Lacombe, C. Le Sech, V. Esaulov, Phys. Med. Biol. **49** (2004) N65
[4] J. de Vries, R. Hoekstra, R. Morgenstern and T. Schlathölter, PRL **91** (2003) 053401
[5] S. Bari, P. Sobocinski, J. Postma, F. Alvarado, V. Bernigaud, B. Manil, J. Rangama, B. Huber, T. Schlathölter, JCP **128** (2008) 074306
[6] F. Alvarado, S. Bari, R. Hoekstra and T. Schlathölter, PCCP **8** (2006) 1922; F. Alvarado, J. Bernard, L. Bin, R. Brédy, L. Chen, R. Hoekstra, S. Martin, T. Schlathölter, ChemPhysChem **9** (2008)
[7] T. Schlathölter, F. Alvarado, S. Bari, A. Lecointre, R. Hoekstra, V. Bernigaud, B. Manil, J. Rangama, B. Huber, ChemPhysChem **7** (2006) 2339