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Electron-induced ionization of DNA components

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Synopsis Ionization of biomolecules remains still today rarely investigated both experimentally and theoretically. In this context, the present work appears as one of the first quantum mechanical approaches providing a multi-differential description of the electron-induced ionization process of the main DNA components for impact energies ranging from the target ionization threshold up to about 10 keV. The cross section calculations are here performed within the 1st Born approximation framework in which the ejected electron is described by a Coulomb wave whereas the incident and the scattered electrons are both described by a plane wave.

Complex DNA lesions including clustered damages have been nowadays clearly identified as the most relevant precursors of elementary steps leading to critical biological lesions like chromosomal aberrations, genome mutagenesis as well as cellular death. Under these conditions and considering that the radio-induced damages in the genome of the living cells are - for about one third - due to the direct attack of the charged particles on the DNA components (the remaining being attributed to the highly reactive hydroxyl radicals produced by the absorption of the radiation in the surrounding aqueous medium), it clearly appears of prime importance to possess an accurate description of the direct ionization process of such complex biomolecules. However, although considerable progress has been made, the available studies on electron-induced ionization of biomolecules such as isolated DNA nucleobases as well as deoxyribose remain extremely rare in both the theoretical and the experimental approaches.

In this context, the current work appears as one of the first quantum mechanical approaches providing a multi-differential description of the electron-induced ionization process of the main DNA components for impact energies ranging from the target ionization threshold up to about 10 keV. The cross section calculations are here performed within the 1st Born approximation framework in which the ejected electron is described by a Coulomb wave whereas the incident and the scattered electrons are both described by a plane wave. The biological targets of interest, namely, the DNA nucleobases and the sugar-phosphate (SP) backbone, are here described by means of the Gaussian 09 system using the restricted Harthree-Fock method with geometry optimization. The theoretical predictions also obtained have shown a reasonable agreement with the experimental total ionization cross sections while huge discrepancies have been pointed out with existing theoretical models, mainly developed within a semi-classical framework [1-4].

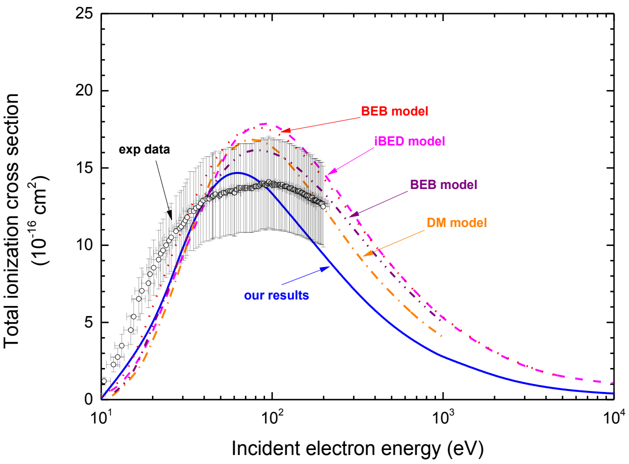

Figure 1. Electron impact total ionization cross section of thymine. Comparison between our results (blue line) [5], classical predictions taken from different sources [1-4] and experimental absolute total ionization cross sections [6].

References

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