Free Electron Production From Nucleotides Upon Collision With Charged Carbon Ions

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Over the last decade Ion Beam Cancer Therapy (IBCT) has become increasingly favored worldwide in the treatment of certain types of cancer. Whereas its effect and usage within cancer therapy is well documented, the understanding of the physical mechanisms behind the therapy is still not entirely understood. The complexity stems from the multiscale nature of the physical phenomena underlying IBCT and span across quantum mechanical to macroscopic scales [1].

The current investigation reports on modelling of the collision process between a highly charged carbon ion and a fragment of a DNA molecule inside a cell. In particular, the quantum mechanical code Octopus 6.0 [2] was employed to simulate the collisions, using a cytosine-guamine nucleotide pair as a representative target. The results suggest that such a collision triggers the release of a large amount of free electrons into the cellular environment, where they might interact with the surrounding medium, possibly creating free radicals or causing direct damage to the DNA. It is furthermore observed that the number of released electrons and the fraction of them that become localized around the carbon ion is highly dependent on the initial kinetic energy of the ion and its impact parameters.

References

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