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On the Need for Theoretical Investigation of Fast-Ion/Biomolecule Interactions

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Treatment of carcinogenic tumors by radiologic means involves, in the ideal case, deposition of energy in a confined volume in order to destroy the reproductive ability of the cancerous cells by destruction of the biomolecular structure of those cells. Concomitantly, as little damage as possible should be done to surrounding tissue. In such treatment, the radiation enters the tissue and transfers its energy to the surrounding tissue, eventually coming to a stop [1]. The Bragg peak (the peak in the energy deposited vs. depth of penetration curve) for radiation penetrating tissue comes at the end of the trajectory for heavy ions, while energy deposition is much more uniform for electromagnetic radiation, x- or γ-radiation. Thus photonic radiation is much more damaging to surrounding tissue than is heavy ion radiation. Consequently, the dose/depth curves are much more favorable for hadronic (heavy ion) than photonic radiation, and recent developments in the treatment of tumors by radiologic means have focused on the use of heavy ion radiation beams such as H^+, He^{2+} and C^{6+}.

The problem then is: How does one predict the best scenario for heavy ion treatment of tumors? To answer that question, an understanding of the details of the interaction of fast ions with various biomolecules (including water!) is imperative. One way to shed some light on this problem is to use today's sophisticated quantum chemical methodology to study heavy-ion/biomolecule interactions under very specific conditions [2].

In order to understand the basic physics of the interaction of heavy ion radiation beams with biomolecules, one needs to understand the characteristics of the interaction as given by such quantities as the cross sections for processes such as fragmentation, ionization, electron transfer, energy deposition, and many others. Although these can all be calculated using the available quantum mechanical tools, the details can be very complicated. For example, if one looks at a very simple case such as collision of fast alpha particles with an isolated nucleobase, and asks for the fragmentation cross section, the questions remain concerning what fragments and with what energy and charge are produced, and in what direction they depart. An advantage of approaching the problem with theory is the details of the initial conditions and resulting situation can be determined with high precision – e.g. there is no uncertainty in beam energy or in fragment ion state. Although experiment can certainly help with this understanding, the details of the understanding of the interaction can only come from theory.

The problem, and its solution, are however, not simple. Biological systems are very complex, and involve many kinds of substances, such as water, protein, DNA and RNA to list a few, in close chemical and physical proximity. They may all interact with a fast hadronic beam, producing a variety of fragments including electrons, free radicals of various sorts, and various ions. The secondary interactions of these fragments with the surrounding environment are then of utmost importance in determination and prediction of the result of the interaction of the beam with particles. Thus the downside of trying to model a very complicated biological system using quantum calculations is that the real system is much more complicated than present day molecular quantum mechanics can handle considering the available computing power.

However, in spite of the difficulties, quantum molecular investigations of the details of hadronic beams interacting with biomolecular targets should be a serious fraction of research involving radiation treatment of tumors. Although experiments must be continued as well, it is the theoretical investigations of individual ion/molecule collisions that will suggest new directions for research and treatment.

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