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Computational investigation of Methacrylic acid as chemical agent for radiation detection by polymerization

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Ion-beam cancer therapy is used for the treatment of cancer. The initial ions in the beam are entering the biological material with energies of a few million eV and are generating secondary electrons by ionization processes. The secondary electrons can cause more ionization or initiate excitation processes, which can cause break some chemical bonds and cause the death of the affected cells. For the adjustment of the dose in ion-beam cancer therapy, it is crucial to have knowledge about these processes. In real biological system this is difficult to achieve, because of the diffusion processes involved.
A methodology, which avoids these problems is the technique of radiation detection by polymerization. In this technique a gel is used, that contains chemical agents, which can polymerize after electronic excitation or ionization. After the irradiation of a probe with the ion-beam, an MRI scanner can be used to locate the distribution of the polymers, which gives an image about the dose distribution. For this purpose the chemical agents in the gel should designed in such a way, that they polymerize at similar energies, at which chemical bonds in biological material (e. g. DNA and amino acids) are broken.
One of the most popular gels for radiation detection by polymerization is MAGIC (methacrylic and ascorbic acid in gelatin initiated by copper) [1]. In our project we want to study the effects energetic electrons on methacrylic acid by means of Monte Carlo simulations [2]. As input parameters the Monte Carlo simulations require the knowledge of cross section data, which describes the various interactions [2]. We will present preliminary results for the cross section for vibrational excitation and ionization, which we have computed with the help of standard quantum chemistry program packages, as described in e. g. [3 - 5].

Bibliography:
[1] M.P. Fong, C. K. Derek, D.D. Mark, J.C. Gore, Polymer gels for magnetic resonance imaging of radiation dose distributions at normal room atmosphere. Phys. Med. Biol. (2001), 46, 3105. DOI: 10.1088/0031-9155/46/12/303
[2] S. Taioli, P. E. Trevisanutto, P. de Vera, S. Simonucci, I. Abril, R. Garcia-Molina, M. Dapor, Relative Role of Physical Mechanisms on Complex Biodamage Induced by Carbon Irradiation. J. Phys. Chem. Lett. (2021), 12, 487–493. DOI: 10.1021/acs.jpclett.0c03250
[3] J. Franz, F. A. Gianturco, I. Baccarelli, Low-energy positron scattering from gas-phase uracil, Eur. Phys. J. D (2014) 68: 183, DOI: 10.1140/epjd/e2014-40796-0
[4] N. F. Lane, The theory of electron-molecule collisions. Rev. Mod. Phys. (1980), 52, 29. DOI: 10.1103/RevModPhys.52.29
[5] W. Hwang, Y.-K. Kim, M. E. Rudd, New model for electron-impact ionization cross sections of molecules, J. Chem. Phys. (1996), 104, 2956 – 2966. DOI: 10.1063/1.471116

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