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Opinion

Computational Nanomaterial Design: Towards the Realization of Nanoparticle Design in Cancer Treatment

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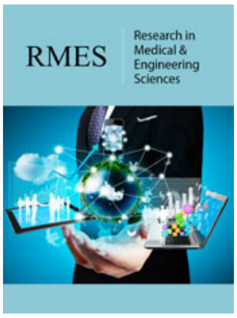

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Opinion

Cancer is one of the leading causes of human mortality [1]. To compound the issue, cancers can occur in many parts of the human body. A new methodology was developed to use radiotherapy to kill cancer cells or control its growth. There are two ways of using this method: external radiation, in which radiation in the form of x-rays bombards the target area from the outside, and internal radiation, in which a small amount of radioactive substance is surgically placed in the vicinity of the cancer cells [2]. Normally, the former method is used for treatment, but this can potentially affect non-cancerous cells and can cause side effects and other unintended problems later on.

The development of nanoparticle technology has increased the amount of arsenal that can be used to treat cancer cells. Among them, gold nanoparticles are most fitting due to its biocompatibility as well as the many advantageous characteristics that can be used against cancer cells [3-12]. Recently, a new development is put forward to combine radiotherapy with nanoparticles in order to be inserted into the patients and operate from inside. While internal radiation has been used before, it relies on the knowledge of the location of the cancer cells in order for the medical personnel to implant the radioactive substances inside the patient. With the radioactive substances being placed on the nanoparticles, along with other targeting components, they can be left on its own devices to target specific cancer cells that these targeting components will bind onto [12]. This increases the potential of the treatment since it can be used to target metastatic cancer cells, or to hold only a specified dosage of radiation enough to treat the cancer cells.

Research is currently ongoing in the form of new materials and clinical trials to study to efficacy of such combinations. However, during the search of the current field, there are very few studies that pertain to the fundamentals of the combination: i.e., what makes the radioactive material want to bind to the nanoparticle? This question is important since answering it would give us an idea on how to design nanoparticles optimized to hold these radioactive elements for cancer-treatment.

The concept of Computational Materials Design (CMD®) is to find out the fundamental mechanism of the process before designing a methodology to optimize the material for various applications [13]. The use of first principles calculation helps us to virtually design materials with desired characteristics in order to provide the best product that can then be verified by experimentalists before undergoing production. Some examples of CMD® in application are fuel cells [14], hydrogen fuel storage [14-16], NO catalyst [17], and investigation of melanin chemistry [18] among others.

Therefore, we embarked on a simulation of two radioactive elements on gold surface: iodine and astatine. Iodine has a long history particularly due to its connection to treating thyroid cancers and can be ingested to perform internal radiotherapy. This is viable since the body will absorb iodine and store it mostly in the thyroid [19]. The second element is astatine. Astatine has attracted attention due to its decay profile of only releasing an alpha particle [20]. Alpha particle is considered the most powerful particle to break the DNA of the cancer cell and therefore disrupt its ability to perform cell division [21-23]. Many experiments and clinical trials have been performed that show the capability of gold nanoparticles to retain these radioactive substances but there are very few explanations on how these elements can stay on the gold nanoparticle [24-27].

Based on our calculations, we found that both iodine and astatine bond to the gold surface via covalent bonding, indicated by the hybridization of the valence orbitals of the adsorbates and gold. This is interesting since the natural assumption would be that both elements bind to gold by ionic bonding, since iodine and astatine are non-metals and gold is a metal. More detailed simulations showed that the charge transfer between such materials are small, which supports our reasoning.

These initial results should be taken as an encouraging prospect to further our goal of designing gold nanoparticles to facilitate the adsorption of radioactive elements. Various other factors must also be taken into consideration before the design can be completed, but we strongly believe that understanding the fundamental process of adsorption allows us to predict the ideal surface and shape of an optimized gold nanoparticle. Cooperation with experimental groups can further verify our calculation results and produce nanoparticles that have improved adsorption capability to ensure that the radioactive substances stay attached to the nanoparticle.

With the importance of treating cancers, a new promising method can be used to provide a wider range of options for patients. Additionally, these new discoveries can encourage the development of new technologies which hopefully allows humanity to live a better life.

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