Nanoparticles for Cancer Therapy

Other

NANOPARTICLES FOR CANCER THERAPY

Tuning Their Shape, Size, and Material using Computer Simulations

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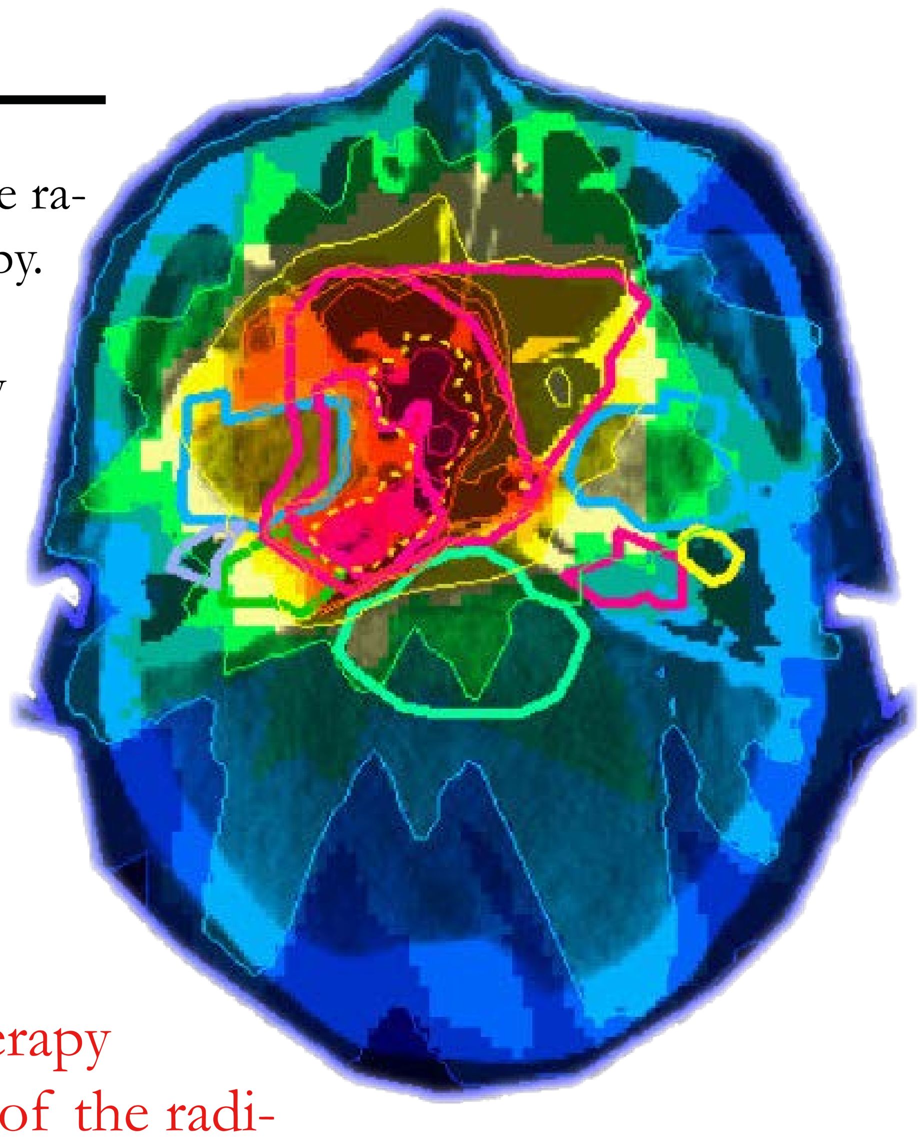
THE PROBLEM



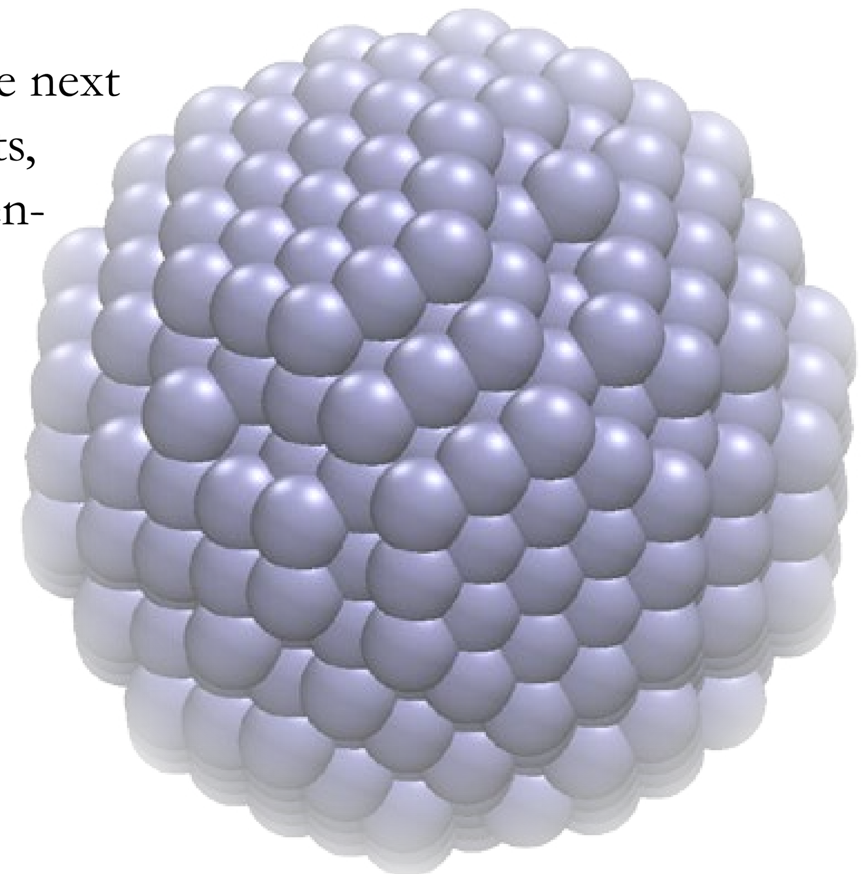
More than 50% of all cancer patients receive radiotherapy which largely means X-ray therapy. X-rays kill cells by the deposition of energy (the "dose") into the cells, but unfortunately these X-rays also damage healthy cells.

Furthermore, radiation is introduced from many angles to increase the dose on the tumor leading to irradiation of much more healthy tissue than strictly necessary - this can be detrimental, especially for brain tumors (see image).

Therefore what is needed is a new therapy that allows more targeted application of the radiation to reduce damage to healthy cells.

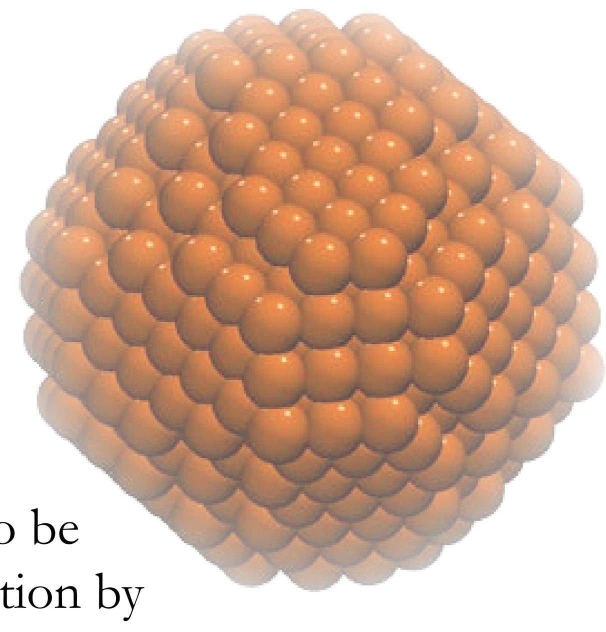
THE SOLUTION

Nanoparticles (particles less than 10 nanometres wide) have been shown to increase the effect of the radiation. This means that less radiation can be used while still achieving the same therapeutic effect.
Less overall radiation => less damage to healthy tissue !



Nanoparticles are regarded as the next generation of radiotherapy agents, but the method by which they sensitize radiation is complex and more research is needed to understand the process and tailor the nanoparticles.

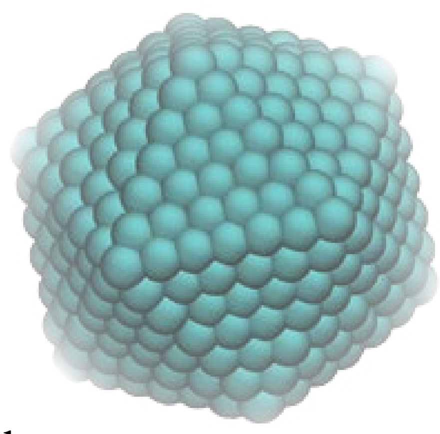
MY PROJECT



As part of a large European project (ARGENT) to explore and develop the use of nanoparticles as the next generation radiotherapeutic agents, I am designing computer simulations to simulate the interaction between nanoparticles, radiation, and cells.
I will be using Molecular Dynamics and Density Functional Theory for the simulations.

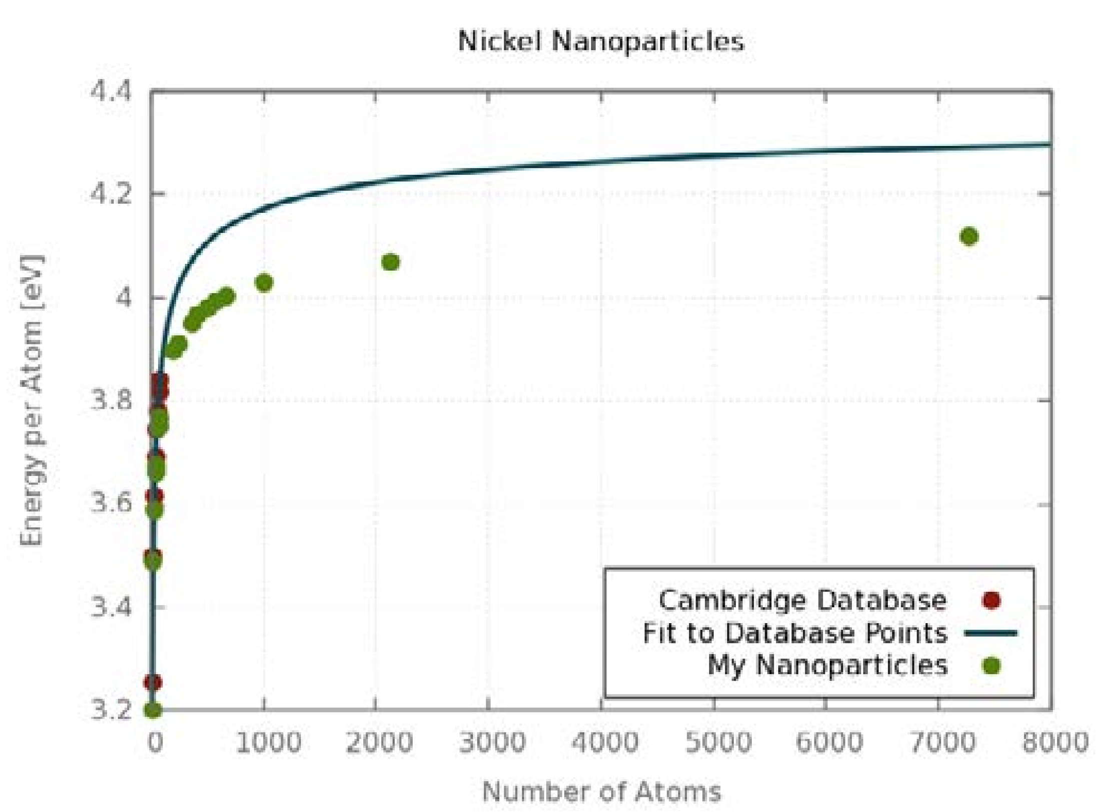
The goal is to find the best shape, size, and material of nanoparticles that will allow them to be successfully incorporated into the tumor cells and increase tumor cell death through irradiation by conventional (X-rays) and next generation radiation (e.g. carbon ions) therapy.

TRUSTING COMPUTERS



A major concern in using computer simulations is whether the computer model is realistic. Therefore in my project I have to show that the model matches reality !
The first step is to be sure that the simulation creates realistic-looking nanoparticles. This is done by modeling the structure of the nanoparticle which in physics parlance means computing the most stable energy configuration.

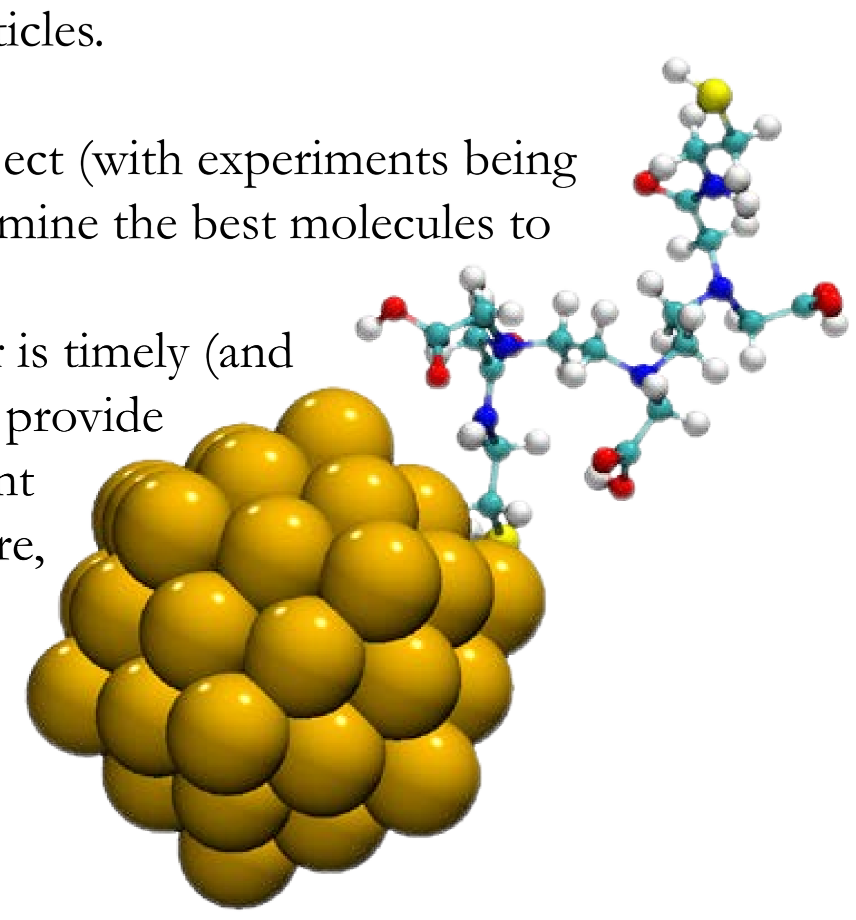
Here, I compare my nanoparticles with those previously computed and stored in The Cambridge Cluster Database - an online collection of optimal structures of nanoparticles of different sizes.



A LITTLE EXTRA ON TOP

Nanoparticles can be guided to cancer cells by attaching specific molecules onto their surface. This also helps avoid strong immune defense reactions to the nanoparticles.

A key part of the ARGENT project (with experiments being performed at the OU) is to determine the best molecules to attach to nanoparticles.
Since experimental trial and error is timely (and expensive) computer simulations provide a tool for exploring many different options. One example, shown here, is the molecule DTDTPA (an organic acid) attached to a small gold nanoparticle.



This project is part of the ARGENT consortium - a Marie Curie funded international project with a total of 13 early stage researchers across Europe working together with academia and industry.
See more on www.itn-argent.eu