Use of Density Functional Theory to determine cross sections for elastic scattering of ions in water

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Abstract
This project aims to combine Density Functional Theory (DFT) with classical scattering theory to determine elastic cross sections of protons interacting with water. This cross sections will be used on Monte Carlo simulations of proton interaction with geometrical model of DNA. DFT is used to determine electrostatic potential around a water molecule. This way, the molecular effects in cross section can be taken into account.

Key words: Monte Carlo, Water, Simulation

Introduction
The elastic cross sections are one of the key components for building a Monte Carlo code for simulating energetic ions' interaction with matter. In our project, in which we want to study these particles' interaction with DNA, the chosen medium is water.
This study uses Density Functional Theory to obtain the electrostatic potential around a water molecule. This potential will be introduced in a Classical Mechanics model (Everhart et al.) to determine the effective cross section for elastic scattering of protons in water.

Results and Discussion
In this first stage, we determined electrostatic potential around the isolated molecule, due to the nuclei (V0) and to the electron cloud (Vh). Then, we introduced a proton getting closer with a certain speed and determined the polarization effect on the potential thanks to charged particle. The objective is to estimate the effect of this polarization on the cross section.

Conclusions
The DFT theory and its time-dependent variant allow to obtain the potential around electronic systems, including complex ones. This potential can be combined with classical scattering theory to determine effective elastic cross section when light ions interact with water (biological medium). In the second part of this project, the potential determined here will be used to calculate proton-water elastic cross sections using the Everhart formalism.

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Image 1. Potential due to the nuclei (V0).

Image 2. Total potential

We are using Octopus code for DFT calculations, which allows us to do time-dependent calculations (TD-DFT).