Ab Initio Exploration of Electronic Dynamics Under Fast Ion Irradiation

Abstract for the general public

Radiation therapy (or radiotherapy) is a primary treatment for various types of cancer and a first-line therapy for many patients. The principle of radiotherapy involves delivering a high dose of ionizing radiation to cancerous tissue. This radiation damages the DNA of affected cells, leading to cell death and therapeutic effects. Traditionally, radiation therapy uses high-energy photons (X-rays) as the ionizing radiation. However, since the early 21st century, proton therapy has increasingly been used. In this approach, a beam of high-energy protons targets cancer cells instead of X-rays. The main differences between proton-based and photon-based radiation therapy arise from their distinct energy deposition profiles in tissue. A photon beam loses energy at an almost exponential rate as it penetrates the tissue. Consequently, to reach deeper cancerous tissue, a higher initial dose of radiation is required or multiple radiation angles must be used, which can damage surrounding healthy cells. In contrast, proton beams (and other heavy ion beams) have a different energy deposition profile. Protons initially lose energy at a slow, constant rate, delivering a lower dose of radiation to shallow tissues. As they reach their characteristic penetration depth, protons slow down rapidly and deposit most of their radiation dose in a small, concentrated region known as the Bragg peak. The location of the Bragg peak depends on the initial proton velocity and can be adjusted to minimize damage to surrounding healthy tissue and to tailor the proton beam for each patient based on the type and composition of the affected tissue.

This research project is concerned with theoretical description of proton-matter interactions for proton velocities most relevant for radiation therapy, i.e. in the region of the Bragg peak which corresponds to the maximum of proton energy loss rate (stopping power) as it travels through matter. In this regime, the available theoretical tools break down or become prohibitively computationally costly. The major objective of the project is develop and implement theoretical methods which enable to study electron dynamics induced by high-energy proton beam at attosecond time scales. These methods will be then applied to (i) determine the stopping power of water from first-principles without any reference to experimental data and (ii) study mechanisms of sensitizer activation in protono-dynamic therapy. However, the theoretical models developed in the project are not limited to the aforementioned applications and will be useful in other research fields such as attosecond science or molecular spectroscopy.