A TDDFT-based study on the proton-DNA interaction.

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The interaction of ionizing particles with DNA induces damage in this molecule. This damage may lead to biological effects, as for instance carcinogenesis. The use of heavy charged particles for radiation therapy is growing very fast due to their dosimetric and radiobiological advantages. However, the mechanisms at the atomic level involved in the early stage of this damage are not well understood yet. In this work we present a study on the proton-DNA collision using the Time-Dependent Density Functional Theory (TD-DFT). An isolated DNA nucleotide pair is targeted by a swift proton, with initial kinetic energy of about 4 keV. The real time evolution of the system electronic density is determined through a time-dependent calculation. As spectroscopy is a powerful tool to study the electronic structure of a molecule, we also determined the absorption spectrum before and after the collision in order to see how this interaction affects the optical properties of the target. This procedure is similar to that used in pump-probe spectroscopy where an external potential perturbs the system and the optical properties are measured afterwards. The electron capture by the proton is clearly observed, which is depicted through the time evolution of the charged distribution profiles normal to the projectile incidence direction. Shifts in the absorption peaks are seen due to the rearrangement of the electronic distribution after the impact of the proton.