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Understanding solvation effects on proton irradiation of DNA from RT-TDDFT simulations

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Proton irradiation of DNA is of utmost importance for many fields, from understanding radiation damage in space and Earth to medical applications for cancer treatment. Computer simulations are highly valuable tools for understanding such process, and among these, ab initio simulations employing Real Time - Time Dependent Density Functional Theory (RT-TDDFT) allow to obtain an extremely detailed description of the process down to the electronic and atomistic scale. However, these are computationally demanding due to the required level of theory, which involves simulating in real time the non-adiabatic propagation of the electronic subsystem of the target material, which is why to date these methods have been restricted to DNA systems in absence of water [1], or at most with few solvating molecules. Here we present the results of RT-TDDFT simulations of proton irradiation of a realistic DNA system (i.e. a DNA strand in bulk water) with pre-sampled proton trajectories [2], where we have determined different important aspects of the proton irradiation process such as the stopping power of the system, the hole/excitation distribution, the spatial distribution of the holes in terms of the depopulations of the maximally localized Wannier functions and, more importantly, the influence of the surrounding water molecules. We will show that water is neither a mere spectator on the process nor a simplistic reducing or enhancing agent of the excitation process [3]. Instead, water qualitatively changes the excitation landscape of the proton-irradiated DNA, making the hole population on the different atoms and bonds qualitatively different in the solvated vs. the dry DNA case. This conclusion warns against the usual practice of extrapolating results obtained in dry DNA systems to the actual DNA system in physiological conditions, and indicates that other models for estimating radiation damage in DNA may need to be revisited.

REFERENCES
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