A Simplest-Level Electron Nuclear Dynamics Investigation of Proton Cancer Therapy Reactions: H^+ + DNA/RNA Bases at E_{Lab}= 80 keV

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In this work, we investigate proton ionization of both DNA and RNA bases with the electron nuclear dynamics (END) theory [1,2] at an energy relevant to the Bragg peak, a phenomenon exhibited by ionizing radiation during materials' penetration. Adopting a single-determinantal wavefunction and classical nuclear mechanics, we employ the simplest-level electron nuclear dynamics (SLEND) and also its Kohn-Sham density functional theory realization (SLEND/KSDFT) [2,3]; both methods are time-dependent, non-adiabatic, direct, and variational, and include electron-nuclear coupling terms. In this study, we analyze the one-electron charge-transfer channel and obtain animations of the simulating collisions, charge-transfer probabilities, and one-electron charge-transfer total integral cross sections. Our results compare well with available experimental [4] and theoretical [5,6] data, thus proving the ability of SLEND and SLEND/KSDFT to provide an accurate charge-transfer description. This study also marks the largest systems examined with SLEND or SLEND/KSDFT to date, thereby demonstrating the utility of our group's new code PACE [2].

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