# Symmetry breaking effects in electron nuclear dynamics simulations of ion cancer therapy reactions

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Ion cancer therapy (ICT) is an approved medical treatment that obliterates cancerous tumors with beams of high-energy ions (usually, $H^+$ and $C^{6+}$ ions) [1]. Despite its established clinical use, the reaction mechanisms that underlie ICT are not known in full detail [1]. This limited understanding results from the difficulty of conducting clinical experiments without harming human subjects. To fill this gap in the ICT characterization, we are conducting computer simulations of several ICT reactions with the electron nuclear dynamics (END) method [2]. END is a time-dependent, variational, direct, and non-adiabatic approach to simulate various types of chemical reactions [1,2]. Due to computational costs, we employ the simplest level (SL) version of END (SLEND) which describes the nuclei in terms of classical mechanics and the electrons with a single-determinantal wavefunction in the Thouless representation [2]. SLEND is implemented in the high-performance simulation package PACE [2]. Here, we present various SLEND simulations of ion-molecule reactions that are computationally feasible prototypes for water radiolysis and DNA damage in ICT. These simulations involve both $H^+$ and $C^{6+}$ ions and several target molecules: $C_2H_4$ [3], $H_2O$ [4], $C_2H_2$, uracil, and cytidine. In these studies, we utilize a computational procedure to induce time-dependent symmetry breaking during simulations [3,4]. By introducing a small degree of symmetry breaking into the initial Hartree-Fock state of the reactants; this initial perturbation transforms into a full-blown symmetry breaking by the time of the reactants' collision. Electron-transfer properties from symmetry-breaking simulations compare better with available experimental data [3,4]. Our SLEND simulations predict various reactive process (e.g., projectile scattering, atom substitutions, target fragmentations, and target-to-projectile electron transfers) and dynamical properties (e.g., integral and differential cross sections) in good agreement with experimental data.

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