Abstract Submitted
for the TSS13 Meeting of
The American Physical Society

Electron Nuclear Dynamics Simulations of Proton Collisions with Water in Proton Cancer Therapy JIEUN YOO, Physics Department, Texas Tech University, AUSTIN PRIVETT, CHRISTOPHER STOPERA, JORGE MORALES, Chemistry Department, Texas Tech University — Proton cancer therapy (PCT) uses high-energy proton projectiles to kill cancerous cells. With water composing ~ 70 % of the human body, the main destructive effects of PCT processes include the radiolysis of water due to proton collisions. Water radiolysis products include radicals and ions formed by fragmentations and ionizations, which can cause damage to the DNA of cells. We conducted electron nuclear dynamics (END) simulations of proton collisions with water clusters $(H_2O)_n$ n=1-5, at 100 keV. These clusters represent a progressive approximation to actual bulk water. END is a time-dependent, variational, direct, and non-adiabatic method that simultaneously models the dynamics of electrons and nuclei in a molecular system. In its current implementation, END uses a classical description for the nuclear degrees of freedom and a single determinant quantum mechanical description for the electronic degrees of freedom. We conducted END simulations revealing mechanistic details and calculated cluster-to-proton electron-transfer integral cross sections (ICSs). Comparison of those ICSs with experimental results involving single water molecules shows good agreement.

Jieun Yoo
Physics Department, Texas Tech University

Date submitted: 01 Mar 2013 Electronic form version 1.4