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The role of multiple ionization in fast highly charged ions collisions on H_2O

N Bachi[1] *, G S Otero[1], S Otranto[1] and R E Olson[2]

[1]Instituto de Física del Sur (IFISUR), Departamento de Física, Universidad Nacional del Sur (UNS), CONICET, Av. L. N. Alem 1253, B8000CPB-Bahía Blanca, Argentina
[2]Physics Department, Missouri University of Science and Technology, Rolla MO 65409, USA

Synopsis An adaptive classical trajectory Monte Carlo model that explicitly considers the eight electrons corresponding to the valence molecular orbitals of the H_2O molecule is introduced. In this dynamical model, the electrons' binding energies change throughout the collision ensuring the proper energy deposition by the projectile for multiple electron removal. Present results are relevant to the ion-therapy program, specially at irradiation planning stages in which detailed information on the electronic emission spectra are needed as input data.

The last few years have seen a steep increase in the number of radiotherapy facilities based on ion beams [1]. This is due to the fact that ion-beam therapy delivers a localized dose of energetic electrons minimizing the unnecessary irradiation of healthy tissue surrounding a tumour. In this context, irradiation planning is an essential tool of the process and is based on numerical simulations which ultimately rely in electron emission cross sections regarding the interaction of the ions of the beam with biological molecular targets.

In this work, we introduce an adaptive classical trajectory Monte Carlo method in which the eight valence electrons of the H_2O molecule are explicitly considered. Although the electronic correlation is not included and screening is only accounted for, electrons' binding energies are changed throughout the collision as the electrons are being emitted. The present method has two clear advantages compared to the independent electrons and sequential electron schemes previously used in the literature [2,3]. First, in the entrance channel the projectile sees the correct electron density and energies. Second, the adaptive scheme ensures that the projectile invests the proper amount of energy in collisional events leading to multiple electron removal.

Singly differential cross sections in energy and angle and recoil charge distributions are studied at an impact energy of 4 MeV/amu for projectiles with charges in the range 1+ to 54+. The electron emission spectra fractions for single and multiple ionization are explicitly determined for the different projectiles under consideration. As a result, we observe that multiple ionization dominates the energetic emission for electron energies greater than about 50 eV.

In Fig. 1 we show the net singly differential cross section in electron emission energy for C^{6+} impact. Our results are compared to the recent experimental data of Bhattacharjee *et al.* [4].

The present methodology is of potential relevance as input data generator for the ion-therapy irradiation simulation codes under use.

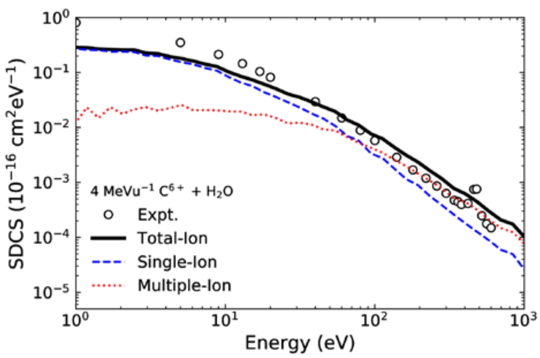

Figure 1. Net singly differential cross section in electron emission energy for 4 MeV/amu C^{6+} + H_2O collisions. The separate contributions from the single ionization and multiple ionization channels are explicitly indicated.

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* E-mail: nicolas.bachi@uns.edu.ar