Single and multiple-electron removal processes from water molecules by H^+ ion impact

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Synopsis We apply the Continuum Distorted Wave-Eikonal Initial State approximation for proton on water-molecule collisions to study multiple electron processes at intermediate to high projectile energy range. Transition probabilities and absolute cross sections were calculated. Results were compared with previous calculations and recent experimental data.

Interaction of charged particles with molecular targets is of fundamental interest in nowadays investigations such as plasma physics [1], thermonuclear fusion [2] and others. In particular, collisions between fully stripped ions and H_2O are of great attention in biology and medicine [3]. Different charge states of the projectile and residual target may be produced as a result of ion-water-molecule interaction. Therefore, it is important calculate pure ionization, capture and transfer-ionization reactions to shed light on the basic mechanisms in multiple electron processes.

The interest of the present work is focused on theoretical calculations of cross sections for single and multiple electron ionization, electron capture and transfer-ionization reactions of water molecules interacting with protons. The three-body Continuum Distorted Wave-Eikonal Initial State approximation (3B-CDW-EIS) [4] is used to calculate transition probabilities (capture and ionization) as a function of the impact parameter and absolute cross sections for the considered collisions. The initial wavefunctions of the active electrons bound to a particular water molecular orbital are described employing the complete neglect of the differential overlap (CNDO) approximation [5]. A trinomial distribution analysis has been employed to compute exclusive probabilities using the independent electron (IEL) model, where electron correlation is neglected [6]. A unitarization procedure is employed to avoid overestimations of 3B-CDW-EIS impact parameter probabilities.

From the comparison with the available theoretical and recent experimental results, we conclude that inclusive probabilities are required for a reliable description of the processes of interest for single-electron removal processes (see Figure 1) and exclusive probability analysis for multiple-electron ones.

The developed approach for calculation of one-electron ionization and capture probabilities allows to investigate multiple electron processes for more complex targets in particular such as macromolecules of DNA and RNA to model scenarios for the radiobiological consequences of the impact of charged energetic particles on those macromolecules.

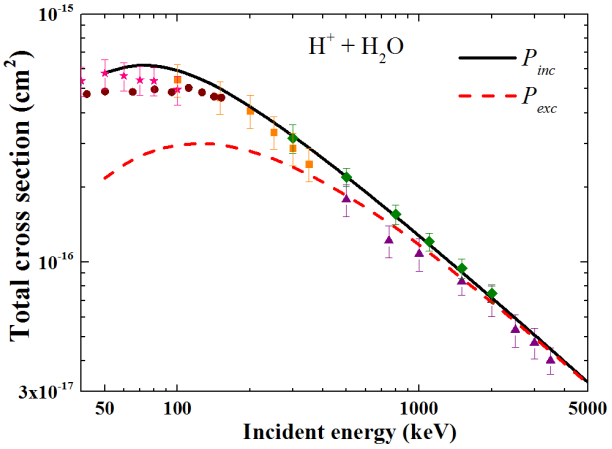

Figure 1. Total single ionization cross sections as a function of the incident energy for H^+ impacting on H_2O.

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