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A numerical lattice approach for ionization and capture processes in ion-H_2O collisions.

L. Errea[1], **Clara Illescas**[2], **L. Méndez**[3], **I. Rabadán**[4], **J. Suárez**[5].

Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain

Synopsis We present a semi-classical numerical integration method for studying electron loss processes in ion collisions with water molecules. Capture and ionization cross section are calculated in the intermediate-high energy range, and the kinetic energy distribution of the ejected electrons is analyzed. The results are compared with those obtained with a classical Monte Carlo method.

Water collisions with ions are relevant in fields such as Astrophysics and Biomedicine. In particular, processes that involve the ejection of electrons play a key role in the biological damage that occurs in ion-beam cancer therapy. Since water is the main component of the cells, there is an increasing demand for detailed information on the ionization of water molecules by ion collisions.

We have carried out non-perturbative, classical and semi-classical, calculations of ionization cross sections in ion-water collisions at impact energies between 10 keV/u and 1 MeV/u, obtaining the kinetic energy distribution of the ejected electrons. The two methods are based on a one-electron approach, where the interaction of the active electron with the core is described by means of a three-center model potential. In both calculations, the projectile follows rectilinear trajectories and the target nuclei remain fixed during the collision. An orientation-averaged cross section is achieved by considering 12 different trajectory orientations. The classical Monte Carlo method has been described in refs. [1, 2].

In this work, we have implemented the direct numerical integration of the Time-Dependent Schrödinger equation in a Cartesian-coordinate lattice scheme. We have adapted the GridTDSE parallel code [3], which was strategically designed with a parallel computational architecture that allows for the massive memory allocations needed in the calculations. The wave function is discretized over a grid of points of the coordinate space, rendering a diagonal potential energy matrix, and the kinetic energy matrix operator is evaluated by applying a finite difference method. We have implemented a Phillips-Kleinman operator [4] to prevent the electron from falling into an occupied orbital of the water molecule. A mask function is introduced at the edge of the grid in order to absorb the ionization and capture fluxes. The kinetic energy distribution of the ejected electrons is obtained from the probability density current at the border of the grid.

Figure 1 shows the probabilities of removing an electron from the $1b_1$ molecular orbital of the water molecule in collisions with protons at $E = 25$ keV and 100 keV.

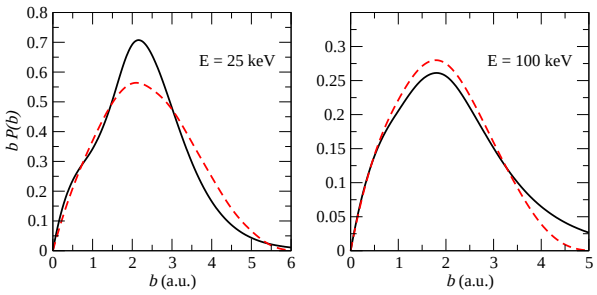

Figure 1. Probabilities for electron dettachment from the $1b_1$ molecular orbital in $H^+ + H_2O$ collisions multiplied by the impact parameter b. (—), numerical results; (- - -), classical results of ref. [1].

References

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[1]E-mail: lf.errea@uam.es
[2]E-mail: clara.illescas@uam.es
[3]E-mail: l.mendez@uam.es
[4]E-mail: ismanuel.rabadan@uam.es
[5]E-mail: jaime.suarez@uam.es