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Calculation of ionization of H_2O by H^+ with classical and semiclassical methods

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Synopsis Total and singly differential (in the electron energy) cross section of electron emission in proton collisions with H_2O are obtained at energies in the range 10 keV to 5 MeV. Two non-perturbative methods are employed, one classical and one semiclassical, both combining a multi-center target electron potential and an independent particle statistics. Excellent agreement with experimental results is found.

The ionization of water molecules by colliding ions is a fundamental process in the description of the interaction of ion beams with biological environments. Since water is the main constituent of the cell, the biological damage is caused, to a large extent, by secondary particles (electrons, ions and radicals) formed by ion collisions with H_2O; accurate cross sections for these atomic processes are therefore required to simulate the passage of ions through biological environments.

While perturbative methods are adept at describing the high-energy collisional regime, non-perturbative methods are necessary to study the ionization process to energies as low as 10 keV. In a recent work [1], we have applied two simple non-perturbative, monoelectronic methods, one classical [2] and one semiclassical [3], to study the ionization of water molecules by proton impact.

Our methods assume:

1. The water nuclei are fixed in their equilibrium positions and the projectile follows rectilinear trajectories.

2. The target molecule is described by means of a multicenter monoelectronic potential. Multielectron probabilities are obtained using an independent particle model.

3. In the CTMC calculation, each molecular orbital is represented by means of a microcanonical classical distribution function $\rho_k(\boldsymbol{r}, \boldsymbol{p})$, build out of $N(\approx 10^5)$ trajectories with the same energy E_k. In the semiclassical method, the scattering wavefunction is expanded in terms of asymptotic frozen fragment molecular and atomic orbitals.

4. Orientation independent cross sections are evaluated by averaging over 12 projectile-target families of trajectories.

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Total and singly differential ionization cross sections are obtained in a wide energy range that goes from 10 keV to 5 MeV. The accompanying figure shows the singly differential electron production cross section (SDCS), obtained with our two methods [1], compared with previous experimental measurements [4, 5] and theoretical [6] data at two projectile energies.

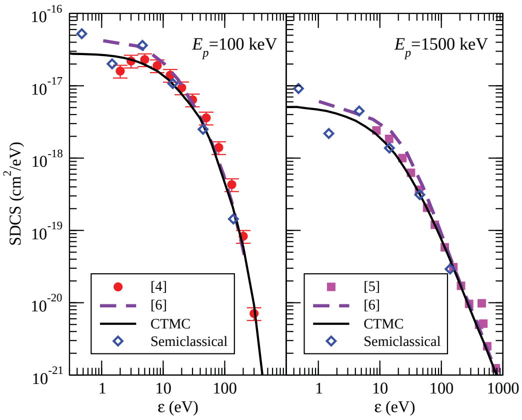

Figure 1. SDCS for electron production in H^++H_2O collisions as functions of the energy of the emitted electron. CTMC and semiclassical results: [1]; experiments:[4, 5]; other theory: [6]. The projectile energy E_p is indicated in each panel.

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