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Influence of the description of the initial bound wavefunction in the single ionization reaction of H₂O molecules

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Synopsis Single ionization of water molecules is considered. Influence of the description of the bound wavefunction and of the continuum states is investigated.

Single electron ionization from water molecules by impact of bare ions is studied. The aim of this work is to investigate the role played by the description of the initial bound and the final continuum states of the emitted electron. To this end, different approaches are employed, within the post and prior version of the CDW-EIS (continuum distorted wave-eikonal initial state) model. In the approximation proposed by Senger *et al.* [1], the double differential cross sections for a given molecular orbital is reduced to a sum of DDCCS related to the atomic orbitals of each atomic compound of the molecule, and the corresponding coefficients are obtained by employing a population analysis within the CNDO approximation. In the calculation of the atomic double differential cross sections, the initial bound wavefunction is described by Slater-type orbitals [2]. In a second approach, we employ the description given by Moccia [3] for the ground state of AH_n-type molecules, where the molecular orbital bound wavefunction is expressed as a weighted sum of Slater-type functions all centered in the heaviest nucleus of the target. Also, an initial molecular three-center wavefunction is considered, being this one obtained as a linear combination of Slater orbitals centered on each target nucleus. The final states are represented by a double product of projectile and target coulomb continuum factors with different effective target charges and a plane wave. These continuum states are chosen within a molecular three-effective center approximation [4].

Double differential cross section (DDCCS) as a function of the energy and angle of the emitted electron were calculated for impact of protons and C⁶⁺ ions on H₂O molecules at intermediate and high collision energies. In these calculations, post and prior versions of the transition amplitude were used. In general, a reasonable agreement with experimental data [5] is obtained. Differences can be observed between post and prior results obtained employing the Senger method, being the last one in better agreement with experiments for both backward and forward emission angles. Concerning the post version, it can be observed that three-effective center results present an enhancement at backward angles with respect to the calculations made with the Senger approach and with the Moccia description, showing a better agreement with experimental data, in particular for the highest electron emission energies.

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