Fully differential cross section calculations for electron impact ionization of methane

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Methane is a greenhouse effect gas and is also employed to simulate organic matter in radiobiology. On a larger scale, methane is an important component of the atmospheres of several planets or moons in our solar system and, presumably, the newly discovered exoplanetary systems may also show the presence of this molecule. These examples clearly emphasize that the interaction between charged particles or other radiation forms and methane is essential from the perspective of several research fields and applications.

Kinematically complete studies have been performed in the last years for the ionization of methane by electron impact both experimentally and theoretically [1-4]. In such studies the physical quantity of interest is the FDCS (fully differential cross section), which provides the most complete information set about the investigated phenomena.

Previously, we have calculated FDCSs for the ionization of several molecular targets by electron impact, including methane [4]. These studies were performed mainly for a coplanar geometry and for intermediate impact energies. In the present study, we investigate the ionization of the methane molecule both in the scattering and perpendicular planes for low energy electrons. Our calculations are performed in the framework of the DWBA (distorted-wave Born approximation) method. The initial state of the molecule is described by Gaussian-type molecular orbitals, while the continuum states are described by distorted waves. The distorted waves are determined in the presence of a spherical potential by averaging the real potential of the nuclei and target electrons. We have performed calculations also for a stronger nuclear potential, by reducing the average C-H distance in order to test the influence of an enhanced nuclei-electron interaction on the cross section. Our results show promising agreement with the experiment, especially in the perpendicular plane. Nevertheless, further investigations are needed in order to correctly describe all aspects of the ionization process.

References:

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