Elastic and Electronically Inelastic Cross sections of H_2 Molecule by Positron Collisions

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Since the initial experimental realizations of positrons, the interest of the scientific community in positron interactions with the matter has increased quickly. The main reason that makes this important antiparticle interesting is due to its wide range of applications. For instance, in material science to identify defects on crystalline structures [1], and medicine in the detection of tumors on the Positron Emission Tomography (PET) [2]. For many of these applications, it is important to obtain data about cross sections of this system. However, despite of these very important applications, the theoretical modeling of inelastic positrons interactions with molecules is still very limited in the literature [3]. Thus, the main goal of this work is to study the effects of the inclusion of electronic excitation in our theoretical modeling of positron-collision processes. For this purpose, we used the H_2 molecule, due to its simple geometric structure and the absence of permanent electric dipole moment. We report theoretical investigation on the elastic and inelastic positron collisions with H_2 molecule for energies up to 50 eV. To compute the elastic and electronically inelastic integral and differential cross sections, we employed the Schwinger multichannel method (SMC). The electronic excited states of molecular target were obtained by employing the configuration interaction method with single excitations (CIS). The Gaussian basis set used to represent the ground and excited states is the same considered in the ref. [4]. Our results were compared to experimental and theoretical elastic and electronic inelastic results available in the literature.

References

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