Double electron capture and electron production in p + Ar collisions

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Synopsis Semiclassical close-coupling molecular expansion and two-electron classical trajectory Monte Carlo methods have been applied to study ionization and capture processes in H^+ + Ar collisions from 100 eV to 400 keV.

Proton - Argon collisions have been studied in many works, however there is a large discrepancy between previous calculations of H^- formation cross sections, which is due to the difficulty of treating the capture of two correlated electrons. In particular, the application of CTMC methods is hindered by the well-known fact that a may-electron atom is classicaly unstable. In a previous work [1], we introduced the switching-CTMC method to classically describe two-active-electron processes in ion-atom collisions. We have applied this method to the treatment of inelastic processes of this system. To cover a large energy range, 100 eV-400 keV, we have also applied a semiclassical treatment with an expansion in a basis of electronic wave functions of the ArH^+ quasimolecule. A block-diagonalization procedure has been implemented to calculate the molecular wavefunctions that dissociate into Ar^{2+} + H^-.

For H formation we find a general good agreement between both methods and the experiments. Classical electron production cross sections are in good agreement with experiments and previous one-electron calculations while the main limitation is the choice of the many-electron interpretation. We will show that the switching-CTMC significantly improves the standard CTMC cross sections for H^- formation showing a better agreement with the measurements. The semiclassical molecular calculation overestimates the experimental cross for H^- formation at $E > 3$ keV (see Fig. 1) because the ionizing flux is trapped in the double capture channels and is the main limitation of this calculation. The workings of both type of methods will be discussed in detail at the Conference.

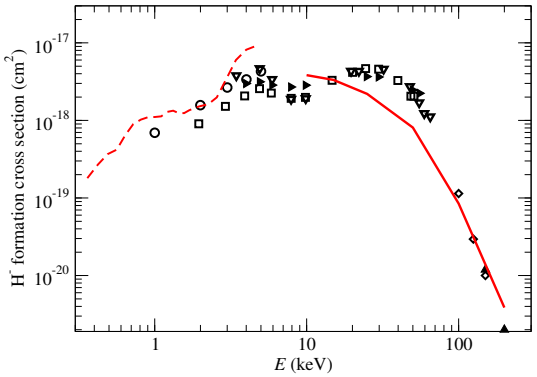

Figure 1. Total cross section for H^- formation as a function of the impact energy. Present results in red lines; different experimental data with symbols (see Ref. [2]).

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References

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[2] Jorge A *et al* 2018 *J. Phys. Chem. A* **122** 2523

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