COLLISION BETWEEN TWO HYDROGEN ATOMS

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Abstract

The interaction in a collision between two hydrogen atoms is studied using the 4-body classical trajectory Monte Carlo method. We present the total cross sections for the dominant channels, namely for single ionization of the target, and ionization of the projectile, resulting from pure ionization and also from electron transfer (capture or loss) processes. We present our cross sections in the projectile energy range between 2.0 keV and 100 keV and compared with them of previously obtained experimental and theoretical results.

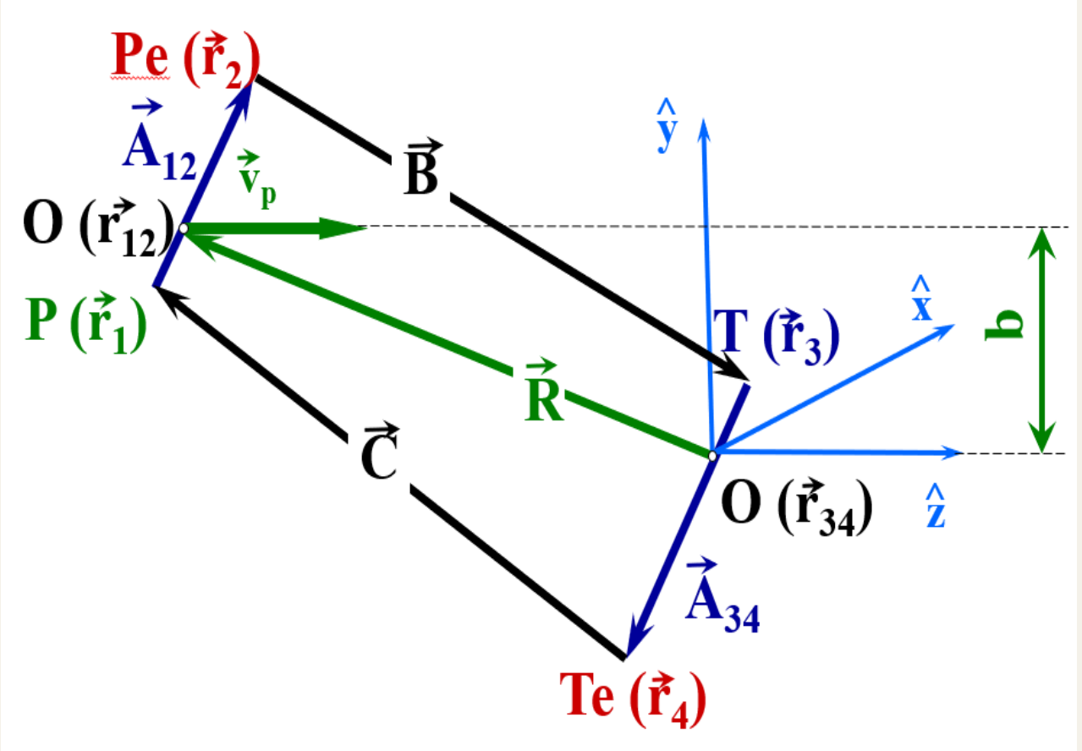
Introduction

Beam emission spectroscopy (BES) is an active plasma diagnostic tool used for density measurements in fusion research. In this technique, a high energy neutral beam of 2.0–100 keV, composed of typically hydrogen atom, light alkali atoms or their isotopes, is injected into the plasma. Through collisional processes with plasma particles, the beam atoms are excited and, subsequently, spontaneous transitions occur, emitting light, which can be observed. Fluctuations in light emission contribute significantly to the study of plasma density fluctuation and related flows. BES codes, modelling the expected light emission from input plasma parameters, require cross section data, such as collisional excitation, de-excitation, charge exchange, and ionization cross sections. Recent plasma research has shifted the focus on the impact of neutrals located at the plasma edge, emphasizing the neutral–neutral collision cross sections, where we have limited data for most of the impact energies or sure from a lack of cross sections. For the case of the collision between two hydrogen atoms, all of the interactions can be exactly taken into account . Here we can take advantage of the classical treatment that, in principle, we do not have any theoretical limit for the number of particles. We can follow all particle trajectories during the collision with the restriction of the classical dynamics.

Theory

In the last two decades there was a great revival of the CTMC calculations applied in atomic collisions involving four or more particles. This approximation seems to be useful in treating atomic collisions where the quantum mechanical ones become very complicated or unfeasible. One of the advantages of the CTMC method is that many-body interactions are exactly taken into account during the collisions on a classical level. The CTMC method is a non-perturbative methods, where classical equations of motions are solved numerically. In the present work the CTMC simulations were made in the 4-body approximation. The four particles (target nucleus, target electron and projectile electron, and projectile nucleus) are characterized by their masses and charges. For the description of the interaction among the particles a Coulomb potential was used.

Classical Method



$$\boldsymbol{H = T + V_C}$$
$$= \frac{\boldsymbol{P_1^2}}{2\boldsymbol{m_1}} + \frac{\boldsymbol{P_3^2}}{2\boldsymbol{m_3}} + \frac{\boldsymbol{P_4^2}}{2\boldsymbol{m_4}} + \frac{\boldsymbol{P_2^2}}{2\boldsymbol{m_2}} + \frac{\boldsymbol{z_4 z_1}}{|\boldsymbol{r_4 - r_1}|} + \frac{\boldsymbol{z_3 z_1}}{|\boldsymbol{r_3 - r_1}|} + \frac{\boldsymbol{z_2 z_1}}{|\boldsymbol{r_1 - r_2}|} + \frac{\boldsymbol{z_4 z_3}}{|\boldsymbol{r_4 - r_3}|} + \frac{\boldsymbol{z_4 z_2}}{|\boldsymbol{r_2 - r_4}|} + \frac{\boldsymbol{z_3 z_2}}{|\boldsymbol{r_3 - r_2}|}$$

$$\text{Hamiltonian Mechanics} \left\{ \begin{array}{l} \dot{\vec{P}}_e = -\dfrac{\delta H_{FMD}}{\delta \vec{r}_e} \\[2mm] \dot{\vec{P}}_T = -\dfrac{\delta H_{FMD}}{\delta \vec{r}_T} \\[2mm] \dot{\vec{P}}_p = -\dfrac{\delta H_{FMD}}{\delta \vec{r}_p} \end{array} \right.$$

$$\ddot{A}_1 = \left[\frac{N_2 z_2 z_1}{\left|\vec{A_1} + \vec{A_2} + \vec{B}\right|^3} + \frac{(N_2 + N_3) z_3\, z_2}{\left|\vec{A_1}\right|^3} + \frac{N_2 z_4 z_2}{\left|\vec{A_1} + \vec{B}\right|^3}\right](\vec{A_1}) + \left[\frac{N_2 z_2 z_1}{\left|\vec{A_1} + \vec{A_2} + \vec{B}\right|^3} - \frac{N_3 z_1 z_3}{\left|\vec{A_2} + \vec{B}\right|^3}\right](\vec{A_2}) + \left[\frac{N_2 z_1 z_2}{\left|\vec{A_1} + \vec{A_2} + \vec{B}\right|^3} + \frac{N_2 z_4 z_2}{\left|\vec{A_1} + \vec{B}\right|^3} + \frac{N_3 z_4 z_3}{\left|\vec{B}\right|^3} - \frac{N_3 z_2 z_1}{\left|\vec{A_2} + \vec{B}\right|^3}\right](\vec{B})$$

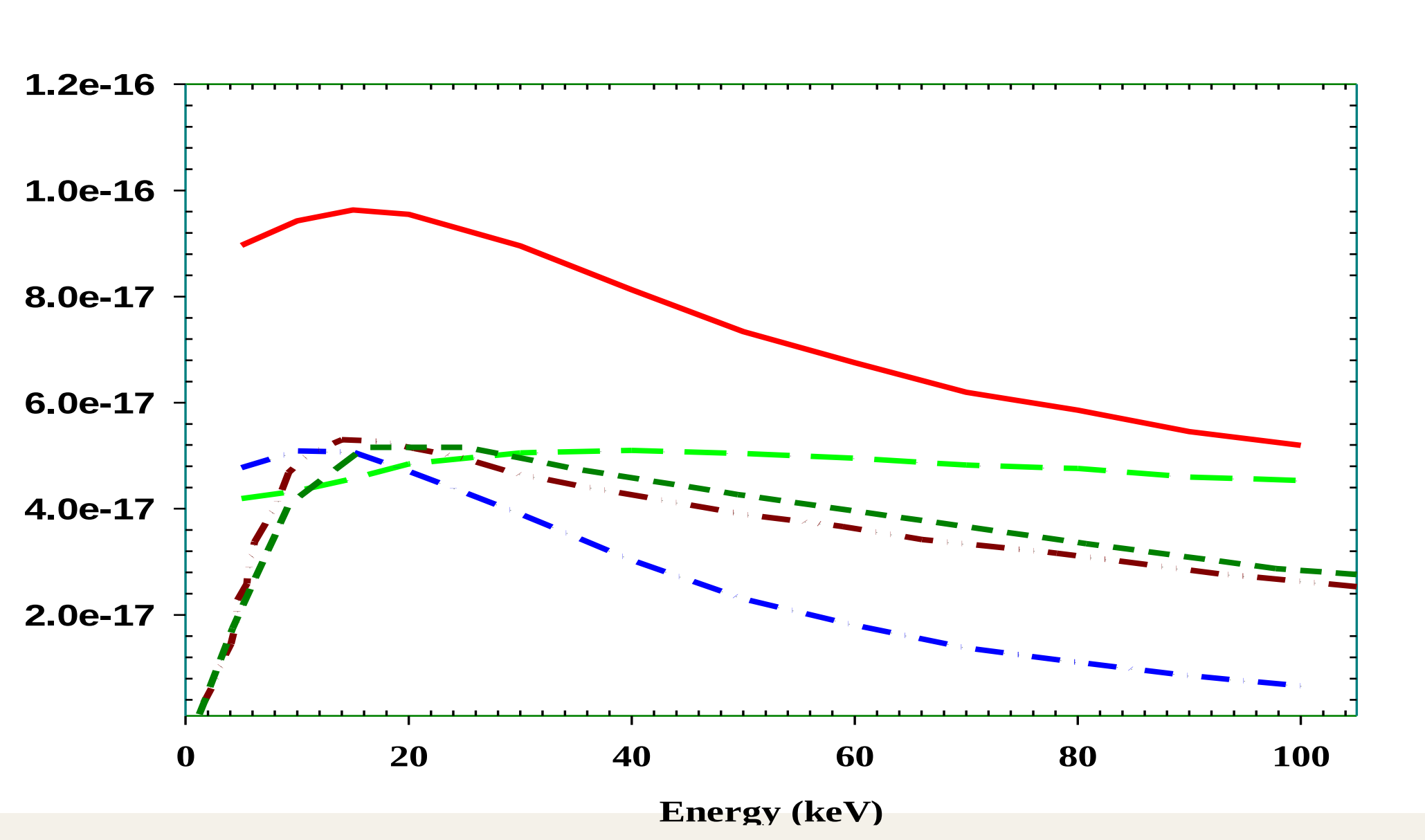
$$\ddot{A}_2 = \left[\frac{N_1 z_2 z_1}{\left|\vec{A_1} + \vec{A_2} + \vec{B}\right|^3} - \frac{N_4 z_4 z_2}{\left|\vec{A_1} + \vec{B}\right|^3}\right](\vec{A_1}) + \left[\frac{(N_4 + N_1) z_4 z_1}{\left|\vec{A_2}\right|^3} + \frac{N_1 z_1 z_3}{\left|\vec{A_2} + \vec{B}\right|^3} + \frac{N_1 z_2 z_1}{\left|\vec{A_1} + \vec{A_2} + \vec{B}\right|^3}\right](\vec{A_2}) + \left[\frac{N_1 z_1 z_2}{\left|\vec{A_1} + \vec{A_2} + \vec{B}\right|^3} - \frac{N_4 z_4 z_3}{\left|\vec{B}\right|^3} - \frac{N_1 z_1 z_3}{\left|\vec{A_2} + \vec{B}\right|^3} - \frac{N_4 z_2 z_4}{\left|\vec{A_1} + \vec{B}\right|^3}\right](\vec{B})$$

$$\dot{\boldsymbol{B}} = \left[\frac{\boldsymbol{N_4 z_2 z_4}}{\left|\vec{\boldsymbol{A_2}} + \vec{\boldsymbol{B}}\right|^3} - \frac{\boldsymbol{N_3 z_3 z_2}}{\left|\vec{\boldsymbol{A_1}}\right|^3}\right](\vec{\boldsymbol{A_1}}) + \left[\frac{\boldsymbol{N_3 z_1 z_3}}{\left|\vec{\boldsymbol{A_2}} + \vec{\boldsymbol{B}}\right|^3} - \frac{\boldsymbol{N_4 z_1 z_4}}{\left|\vec{\boldsymbol{A_2}}\right|^3}\right](\vec{\boldsymbol{A_2}}) + \left[\frac{\boldsymbol{N_3 z_1 z_3}}{\left|\vec{\boldsymbol{A_2}} + \vec{\boldsymbol{B}}\right|^3} + \frac{\boldsymbol{N_4 z_4 z_3}}{\left|\vec{\boldsymbol{B}}\right|^3} + \frac{\boldsymbol{N_4 z_2 z_4}}{\left|\vec{\boldsymbol{A_1}} + \vec{\boldsymbol{B}}\right|^3}\right](\vec{\boldsymbol{B}})$$

Results I

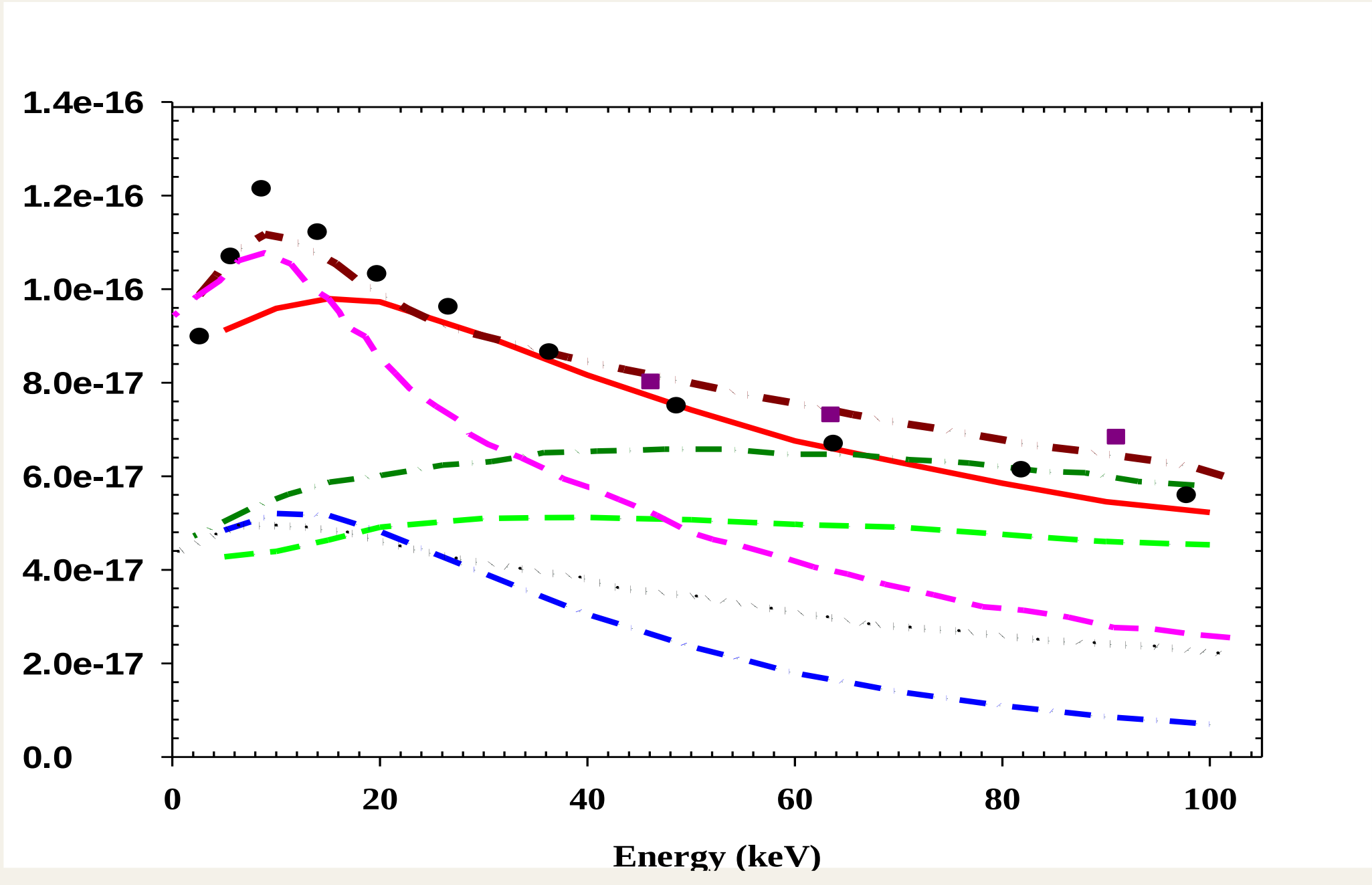
Target Ionization

$$(\boldsymbol{H_P^+, e_P^-}) + ((\boldsymbol{H_T^+, e_T^-}) \rightarrow (\boldsymbol{H_P^+, e_P^-}) + \boldsymbol{H_T^+}, +\boldsymbol{e_T^-}$$



Projectile Ionization

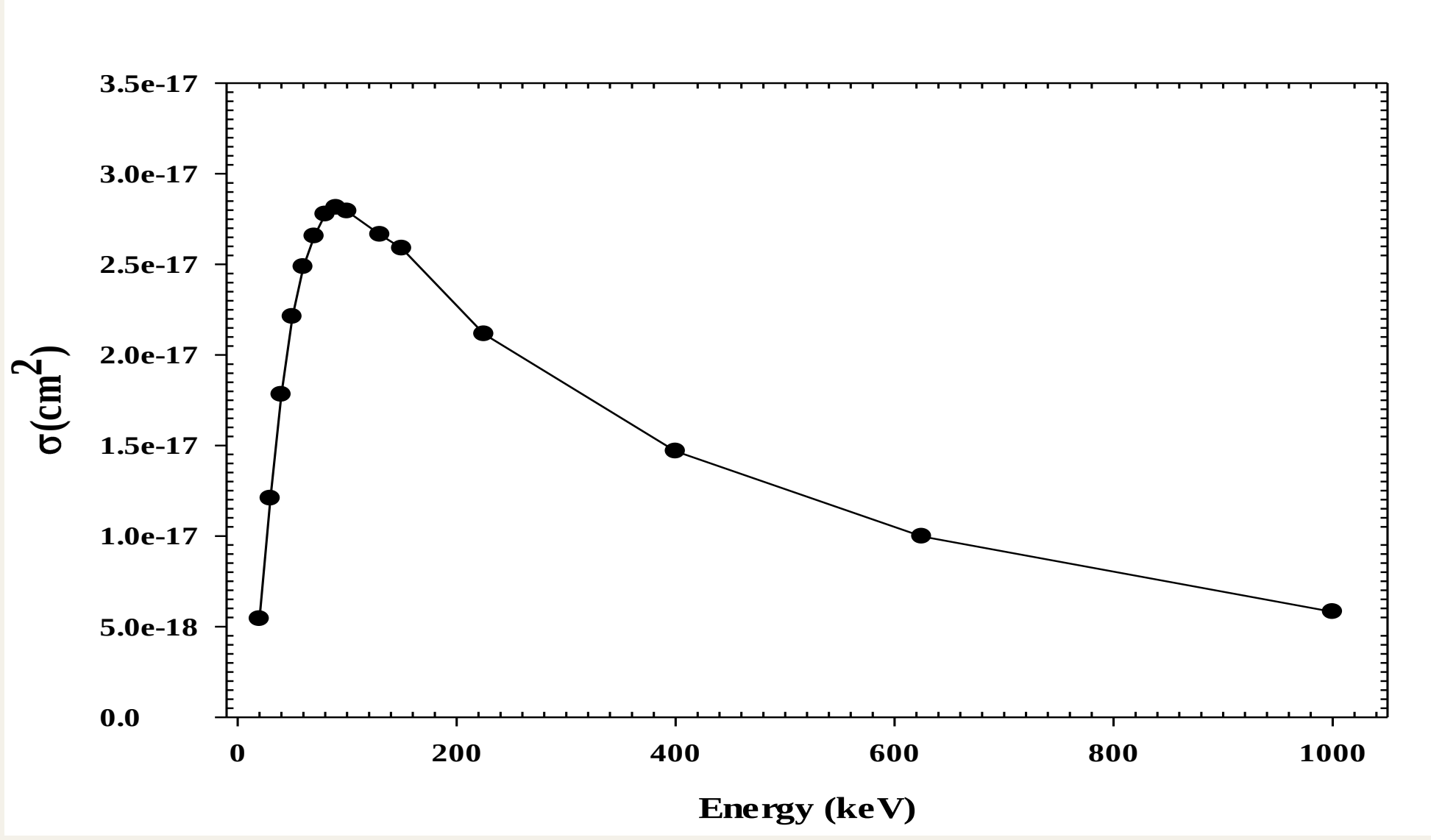
$$(\boldsymbol{H_P^+, e_P^-}) + ((\boldsymbol{H_T^+, e_T^-}) \rightarrow (\boldsymbol{H_T^+, e_T^-}) + \boldsymbol{H_P^+}, +\boldsymbol{e_p^-}$$



Results II

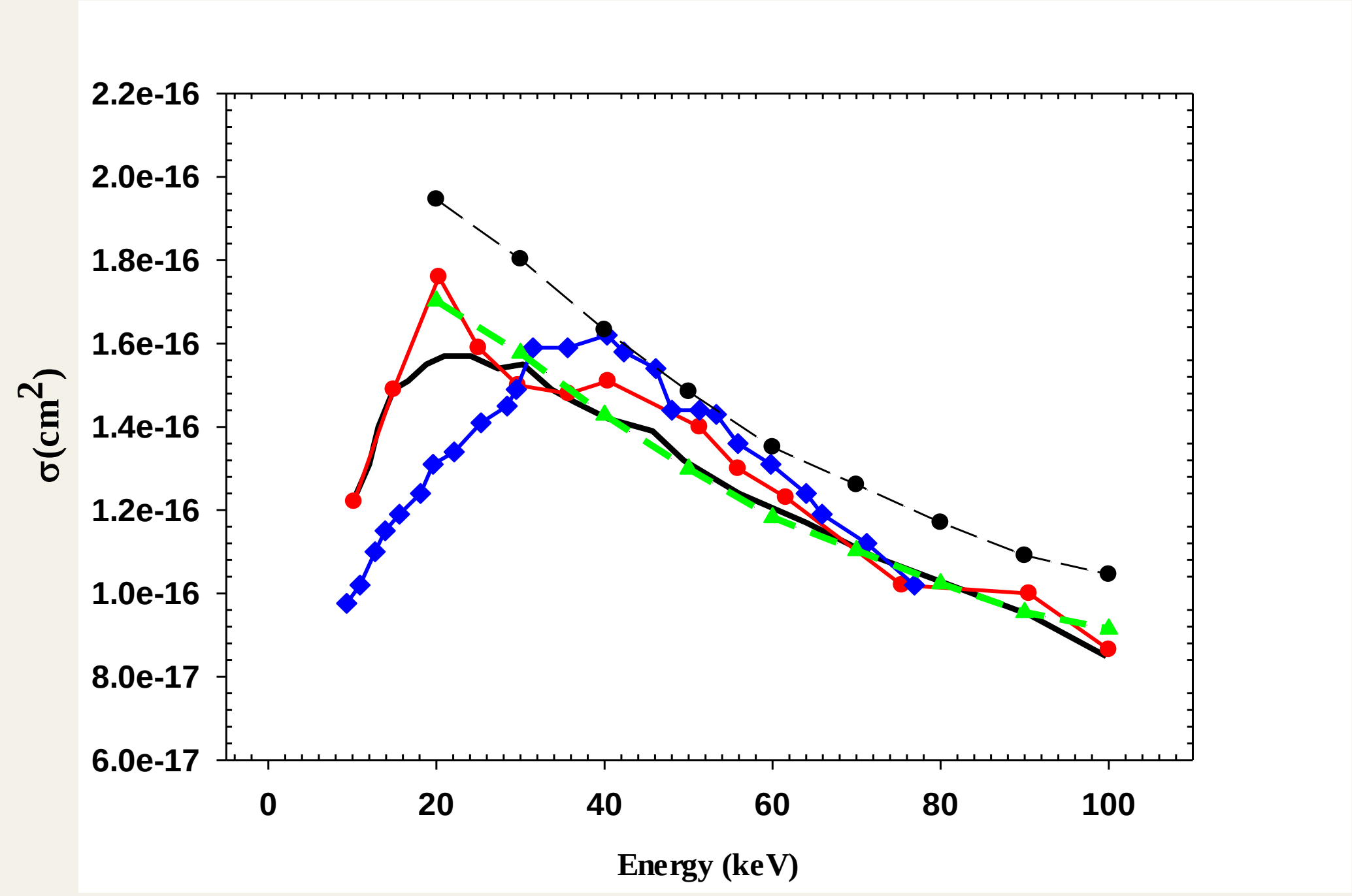
complete break of our system

$$(\boldsymbol{H_P^+, e_P^-}) + ((\boldsymbol{H_T^+, e_T^-}) \rightarrow \boldsymbol{H_P^+} + \boldsymbol{e_P^-} + \boldsymbol{H_T^+}, +\boldsymbol{e_T^-}$$



Target Ionization

$$(\boldsymbol{H_P^+, e_P^-}) + ((\boldsymbol{H_T^+, e_T^-}) \rightarrow (\boldsymbol{H_P^+, e_P^-}) + \boldsymbol{H_T^+}, +\boldsymbol{e_T^-}$$



Target ionization cross sections as a function of projectile impact energy. Green dash-line: present CTMC results for H+H collision multiply by 1.75; Black circle with dash-line: present CTMC results for H+H collision multiply by 2; red circle with solid line: experimental data of H+H_2 by Solov'ev et al. 1962; blue diamond with solid line: Schwirzke 1960.

Conclusion

In summary, we presented simulation results in collision between two hydrogen atoms in the ground states using the classical trajectory Monte Carlo method. In our calculations we considered ten million trajectories for each collision system. We have shown that the classical treatment can able to describe reasonable well the calculated cross sections. We found reasonable good agreements with the previous results.

Acknowledgements

The work was support by the National Research, Development and Innovation Office (NKFIH) Grant KH126886. This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission

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