Interaction of lithium atom with hydrogen molecule

K Tőkési[1,2] *, O Asztalos[3], B Szondy[3] and G I Pokol[3,4]

[1]Institute for Nuclear Research, Hungary Academy of Sciences (Atomki), 4001 Debrecen, Hungary
[2]ELI-ALPS, ELI-HU Non-profit Ltd., Dugonics ter 13, H-6720 Szeged, Hungary
[3]Institute of Nuclear Techniques, Budapest University of Technology and Economics, Muegyetem rkpt 3, 1111 Budapest, Hungary
[4]Wigner –RCP, Hungarian Academy of Science, 1121 Konkoly-Thege Miklos 29-33, Budapest,

Synopsis The interaction between lithium atom and hydrogen molecula 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 for wide range of incident velocities of the lithium atom. Our results are compared with available previous reults.

Understanding and an accurate description of fusion plasma properties and its diagnostics, requires knowledge of a wide range of particle interactions and cross sections over several magnitudes of impact energies. Although the last decades, it was a trial of a large-scale study to provide this data, still many basic atomic and molecular cross sections are missing.

Along this line, in this work, the interaction between lithium atom and hydrogen molecula is studied using the 4-body classical trajectory Monte Carlo method in wide range of Li impact energies [1].

Interpretation of the cross sections in Li + H_2 collisions is a challenging task for theories. The main difficulty is caused by the many-body feature of the collision, involving the projectile, projectile electron(s), target nucleus, and target electron(s). The classical trajectory Monte Carlo (CTMC) method, however, has been quite successful in dealing with the ionization process in ion-atom collisions. 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 nonperturbativ method, where classical equations of motions are solved numerically. In the present work the CTMC simulations were made in the four-body approximation (see Fig.1.), i.e. the many-electron target atom was replaced by a one-electron atom and the projectile was taken into account also as two particles. H_2 molecule is modeled by a hydrogen-type atom with one active electron bound to the H_2^+ ion with an effective binding energy (E_{eff}) and an effective core nuclear charge (Z_{eff}). We used Z_{eff} = 1.165 and E_{eff} = 0.567 a.u for H_2.

* E-mail: tokesi@atomki.mta.hu

This type of two body approximation was successfully applied in the investigation of the H_2O molecule by several groups, leading to a good agreement between theoretical predictions and experimental data. For the multilectron Li projectile, we take into the 2s electron of the Li atom. The effective charge of 1.3 and binding energy of 0.198 a.u.were used to model the 2s orbital of the Li atom.

A large number (10^6) of primiray trajectories were followed based on our four body model. The obtained cross sections were compared with previous data [2].

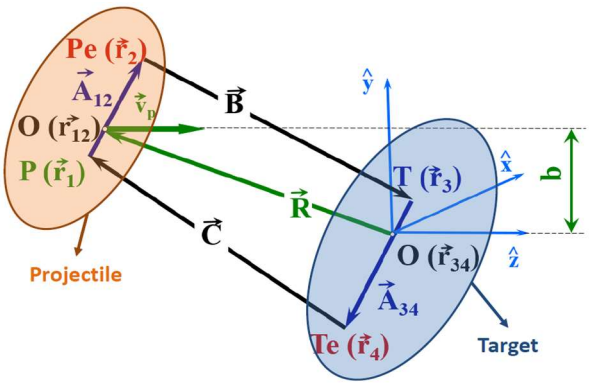

Figure 1. Schematic diagram of the 4 body simulation.

We found that our method is reliable for the generation of nonexistent cross-sections like, excitation, ionization and charge exchange cross sections.

References

[1] Tőkési K *et al* 1994 *Nucl. Instr. Meth. Phys. Res. B* **86** *147*

[2] Wutte D *et al* 1997 At. Data Nucl. Data Tables **65** 155