Classical simulations of collisions between light particles

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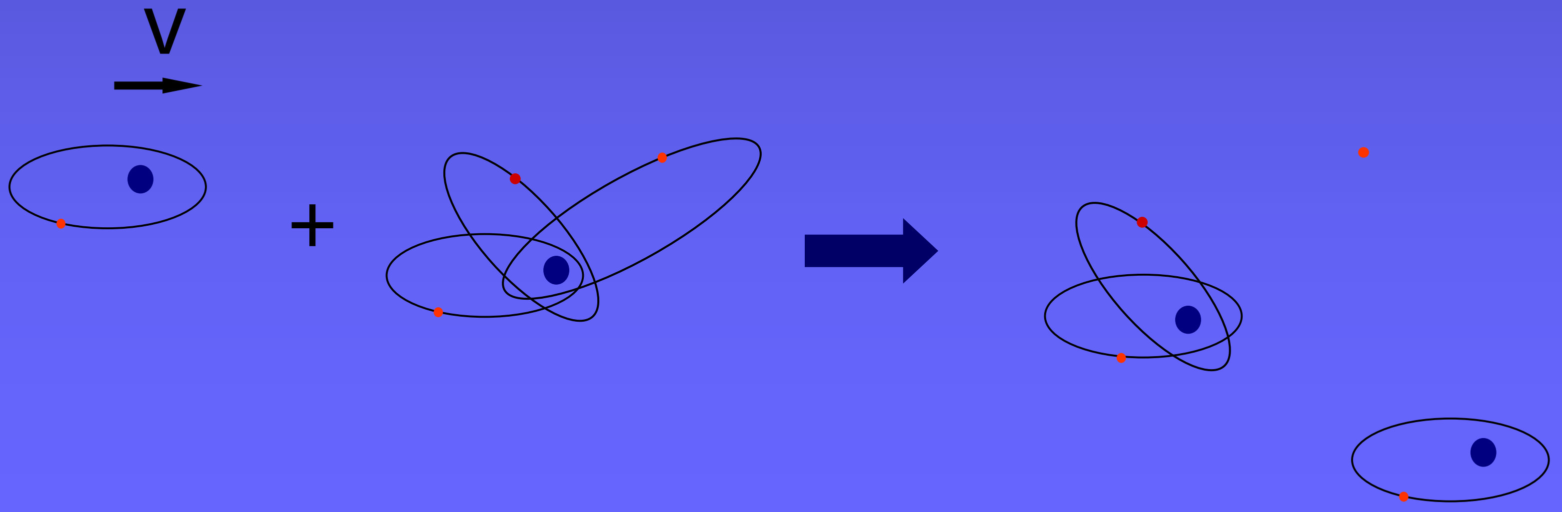

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Institute of Nuclear Techniques, Budapest University of Technology and Economics, Budapest, Hungary

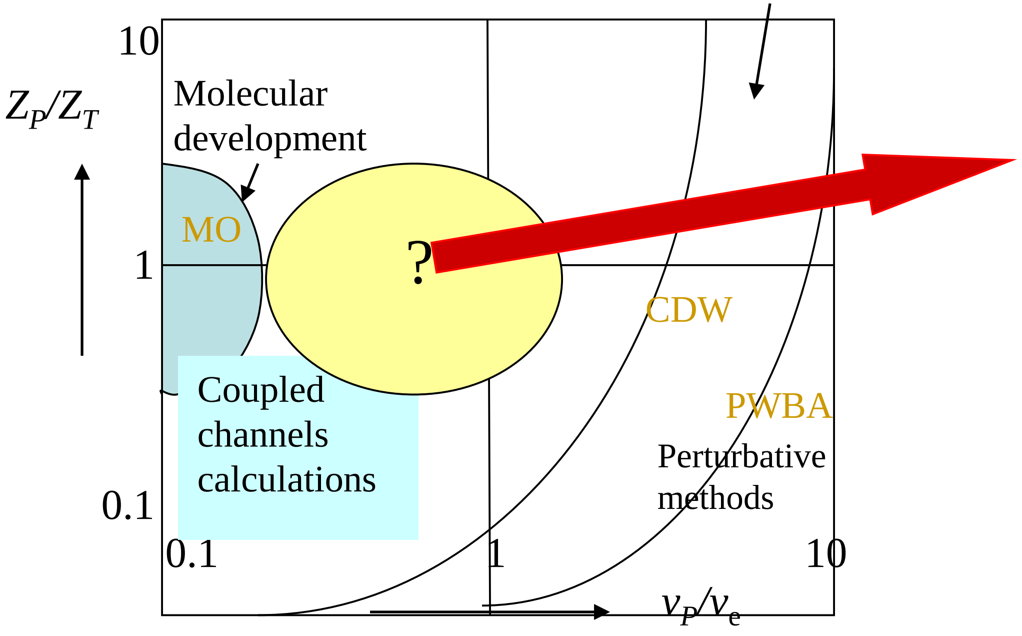
Outlook

- Basic idea
- Classical methods
  CTMC
  - a method of the analysis
- H + H
- Li + H
- $Li^{+} + N_2$ ($e^{+} + N_2$)
- Summary

Ionization in ion-atom collisions

Description:

Distorted wawe approximations



adiabatic

fast

Non-perturbative models:

Classical Trajectory Monte Carlo (CTMC) method

3-body CTMC approach

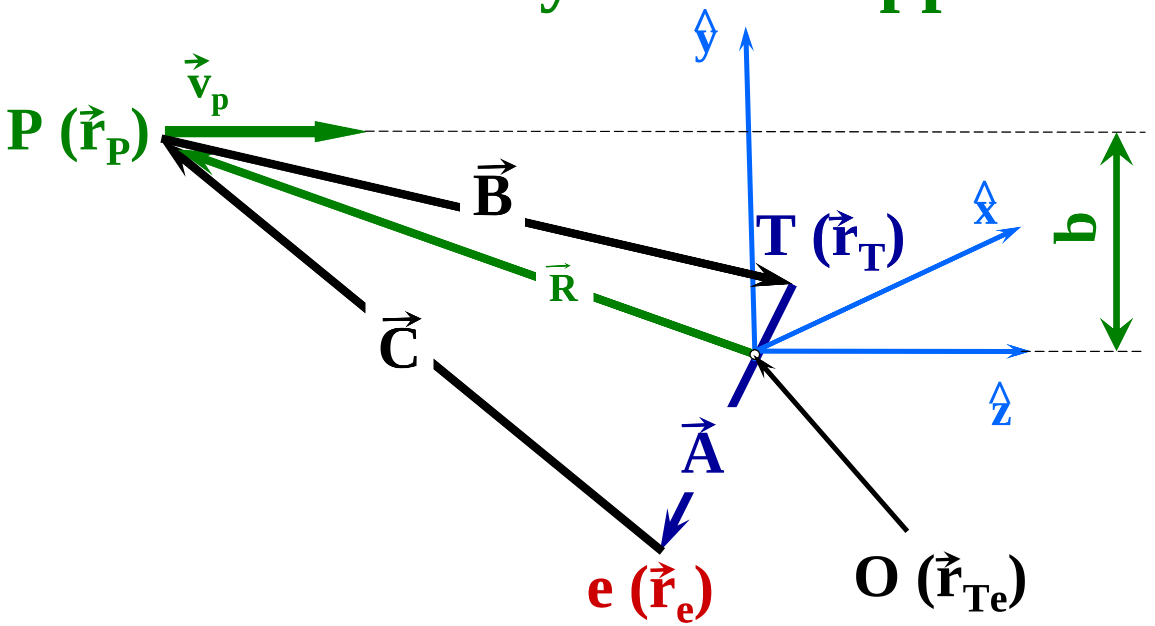


Fig. 1. The relative position vectors of the particles involved in 3-body collisions. $A = \vec{r}_e - \vec{r}_T$, $B = \vec{r}_T - \vec{r}_P$, $\vec{C} = \vec{r}_P - \vec{r}_e$, $\vec{r}_{Te}$ is the position vector of the centre-of-mass of the target system, and b is the impact parameter.

$$L = L_K - L_V$$

$$L_K = \frac{1}{2} m_P \dot{\vec{r}}_P^2 + \frac{1}{2} m_e \dot{\vec{r}}_e^2 + \frac{1}{2} m_T \dot{\vec{r}}_T^2$$

$$L_V = \frac{Z_P(|\vec{r}_P - \vec{r}_e|) Z_e}{|\vec{r}_P - \vec{r}_e|} + \frac{Z_P(|\vec{r}_P - \vec{r}_T|) Z_T(|\vec{r}_P - \vec{r}_T|)}{|\vec{r}_P - \vec{r}_T|} + \frac{Z_e Z_T(|\vec{r}_e - \vec{r}_T|)}{|\vec{r}_e - \vec{r}_T|}$$

Exist test in 3-body CTMC simulation

	Direct process	Ionization	Charge transfer
E_{Te}	**<0**	**>0**	**>0**
E_{Pe}	**>0**	**>0**	**<0**

$$\ddot{\vec{A}} = \left[\frac{(N_2 + N_3) Z_2 Z_3}{\left|\vec{A}\right|^3} + \frac{N_2 Z_1 Z_2}{\left|\vec{A} + \vec{B}\right|^3} \right] \vec{A} + \left[\frac{N_2 Z_1 Z_2}{\left|\vec{A} + \vec{B}\right|^3} - \frac{N_3 Z_1 Z_3}{\left|\vec{B}\right|^3} \right] \vec{B}$$

$$\ddot{\vec{B}} = \left[-\frac{N_3 Z_2 Z_3}{\left|\vec{A}\right|^3} + \frac{N_1 Z_1 Z_2}{\left|\vec{A} + \vec{B}\right|^3} \right] \vec{A} + \left[\frac{N_1 Z_1 Z_2}{\left|\vec{A} + \vec{B}\right|^3} + \frac{(N_1 + N_3) Z_1 Z_3}{\left|\vec{B}\right|^3} \right] \vec{B}$$

Classical principal quantum number:

$$n_c = Z\sqrt{\frac{\mu}{2U}}$$

n_c is "quantized" to a specific n [J.Phys.B**17** (1987) 3923]:

$$\left[(n-1)(n-0.5)n\right]^{1/3} \le n_c \le \left[n(n+0.5)(n+1)\right]^{1/3}$$

Classical orbital angular momentum:

$$l_c = \left[(x\dot{y} - y\dot{x})^2 + (x\dot{z} - z\dot{x})^2 + (y\dot{z} - z\dot{y})^2\right]^{1/2}$$

l_c is "quantized" to a specific l:

$$l \le l_c \frac{n}{n_c} \le l+1$$

Cross section:

$$\sigma_{(n,l)} \frac{2\pi b_{\max} \sum_j b_j^{(n,l)}}{N}$$

The total and double differential cross-sections were computed with the following formulas:

$$\sigma = \frac{2\pi b_{\max}}{T_N} \sum_j b_j^{(i)}$$

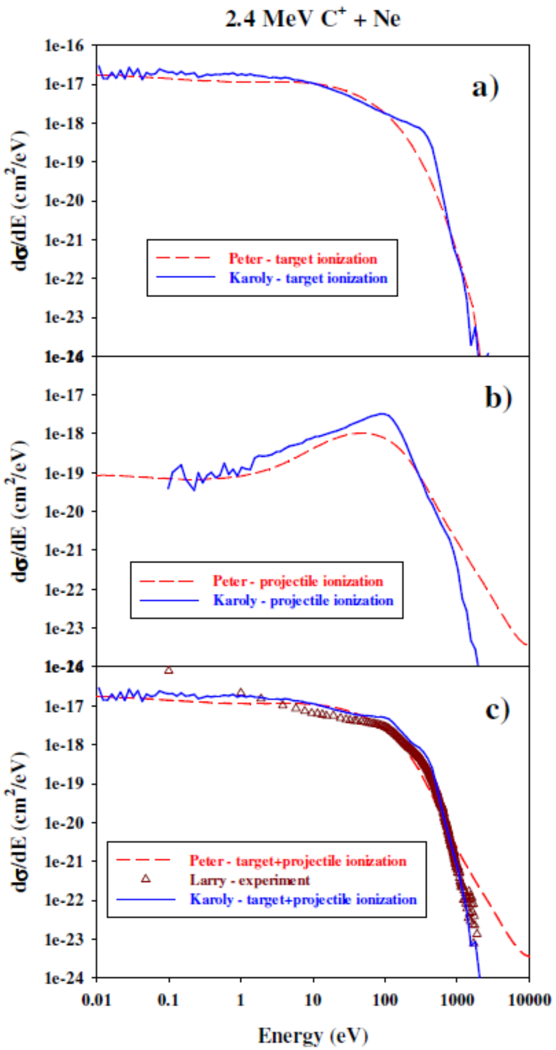
$$\frac{d^2\sigma}{dEd\Omega} = \frac{2\pi b_{\max}}{T_N \Delta E \Delta\Omega} \sum_j b_j^{(i)}$$

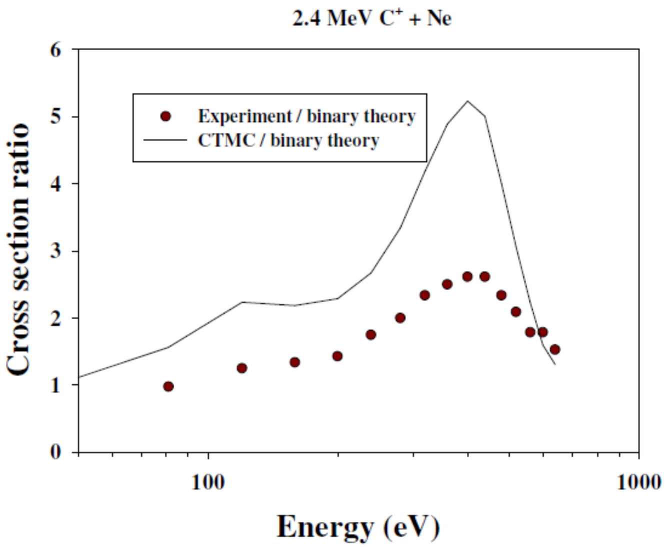
The statistical uncertainty of the cross section is given by

$$\Delta\sigma = \sigma \left(\frac{T_N - T_N^{(i)}}{T_N T_N^{(i)}} \right)^{1/2}$$

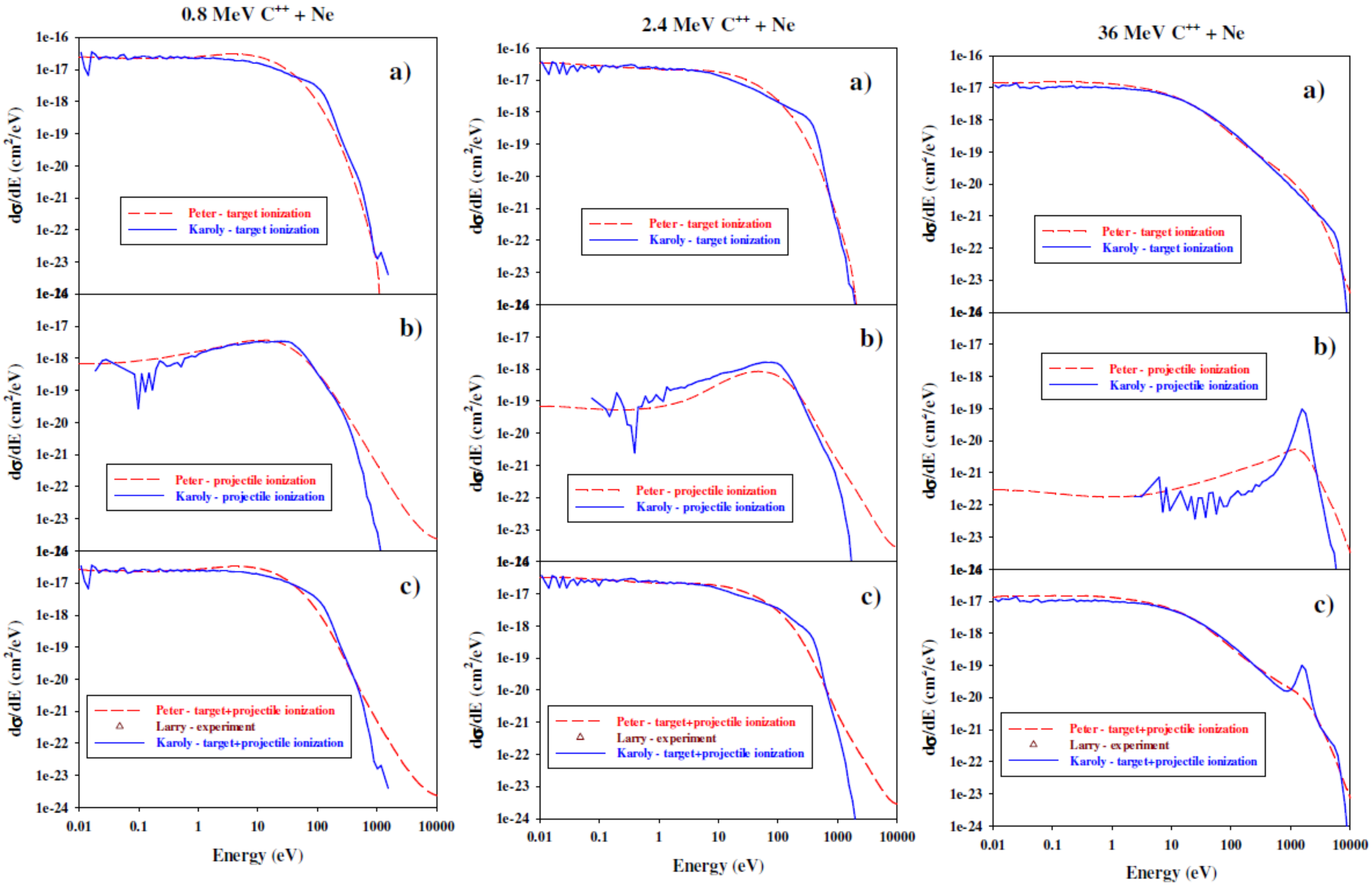
Test -- Interaction of C^+ and C^{++} with Ne

Energiaspektrumok 2.4 MeV C⁺ és Ne ütközésben



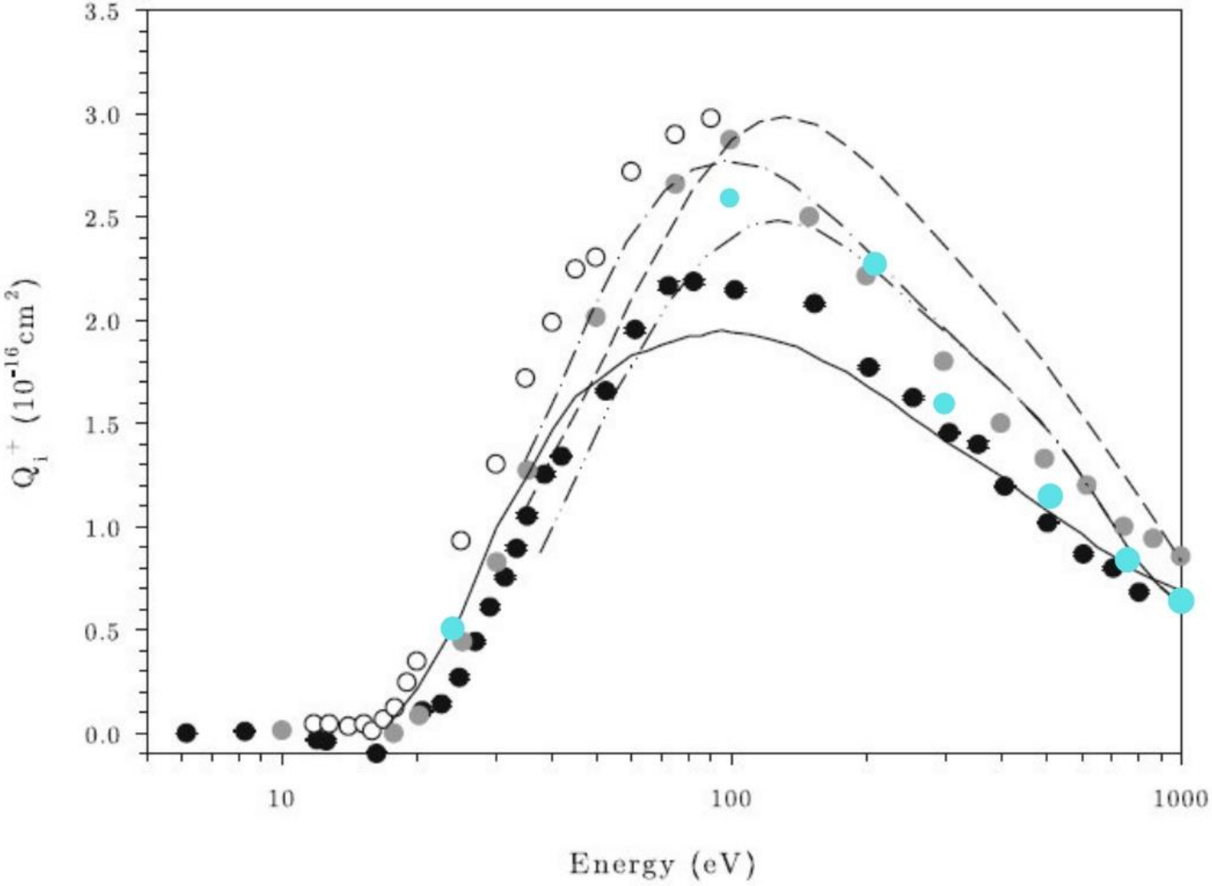


Energia spektrumok C^{++} és Ne ütközésben

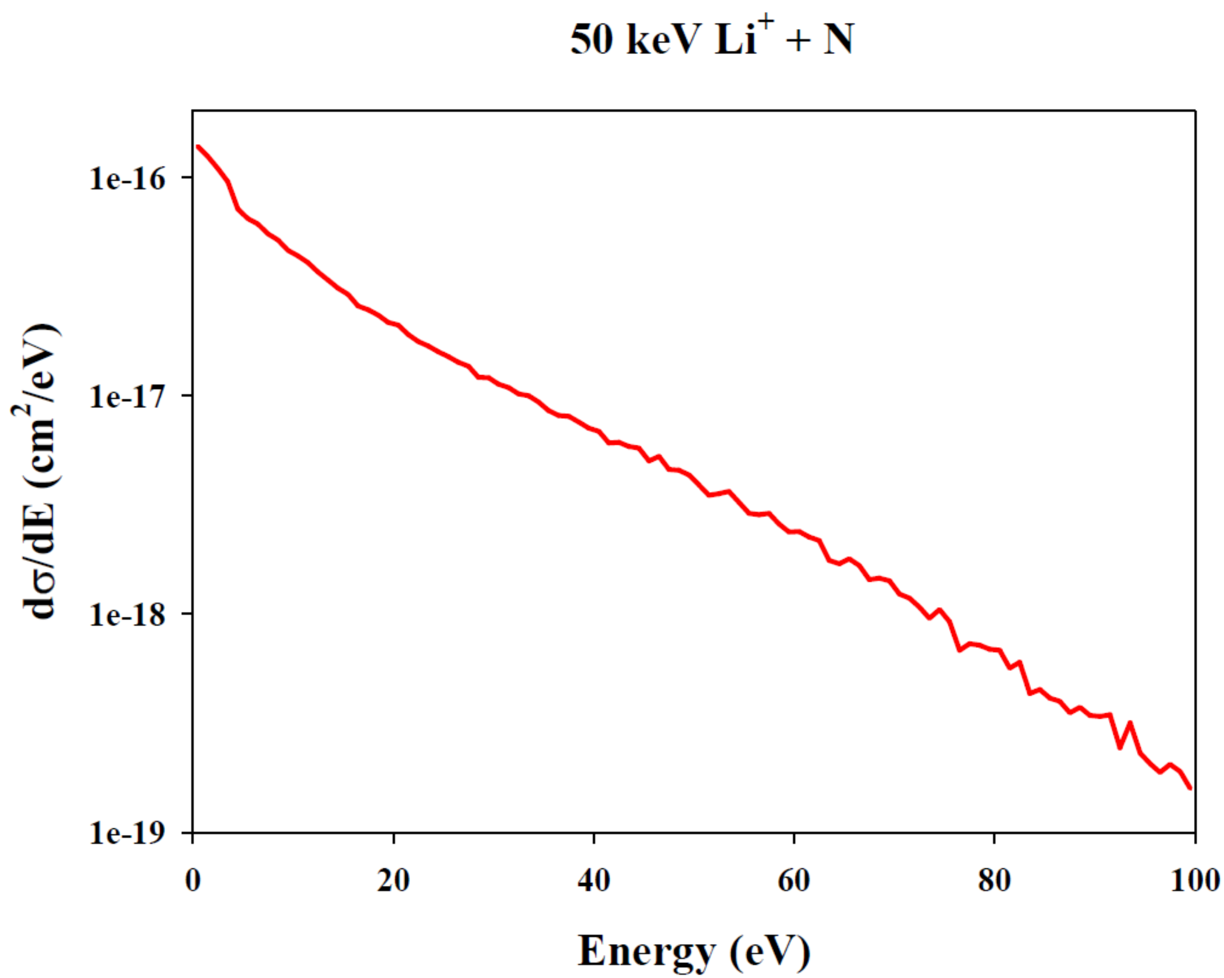


$Li^+ + N_2$

Test of the calculation procedure.
Published data available $e^+ + N_2$

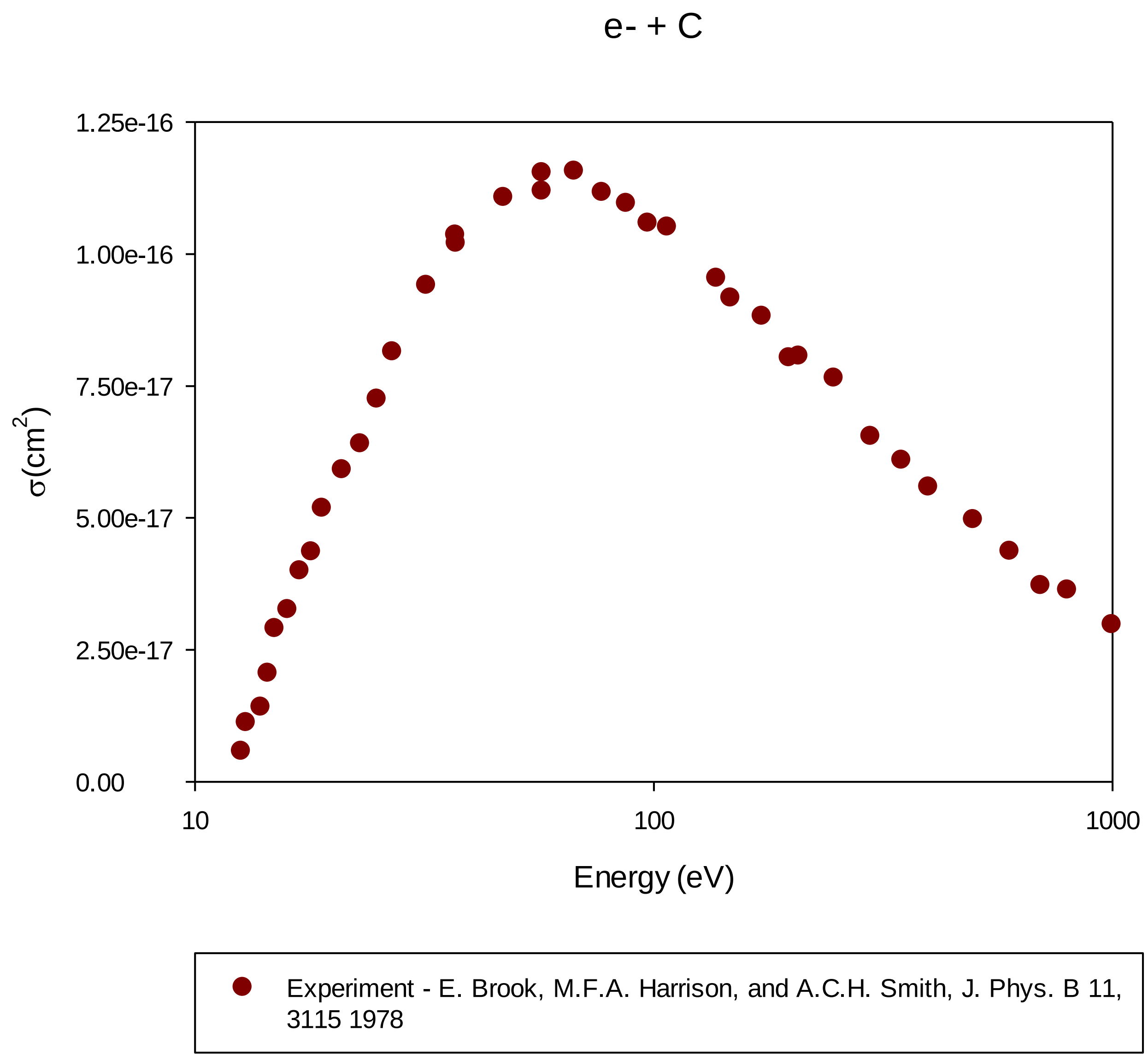


```
                                 Li+ -> N(2p)

                  I D E N T I F I E R =  elasion

     Pm=  0.11016000D+05      Em=  0.10000000D+01     Tm=  0.25704000D+05
     Pz=  0.30000000D+01      Ez= -0.10000000D+01     Tz=  0.70000000D+01
  Ubind= -0.53410000D+00  Rstart=  0.20000000D+03  Rstop=  0.10000000D+04
   B_max=  0.50000000D+01
   V(TE) : coulomb       V(PE) : coulomb       V(TP) : coulomb
          Vp=  0.5776D+00 au.    Ep=  0.5000D+02 KeV

      ntotal current=     9998     ntotal expected=    10000

              direct=     7454               äbiei=  0.20928208D+05
   direct ionization=      436               äbiei=  0.30370774D+03
 transfer ionization=      373               biei=  0.32665284D+03
     charge transfer=     1735               biei=  0.32462153D+04
      anomal trajec.=        2               biei=  0.00000000D+00


              direct= (  0.18402640D-14 +-   0.10751955D-16) cm**2
   direct ionization= (  0.26705699D-16 +-   0.12507730D-17) cm**2
 transfer ionization= (  0.28723313D-16 +-   0.14592305D-17) cm**2
     charge transfer= (  0.28544695D-15 +-   0.62299990D-17) cm**2
```

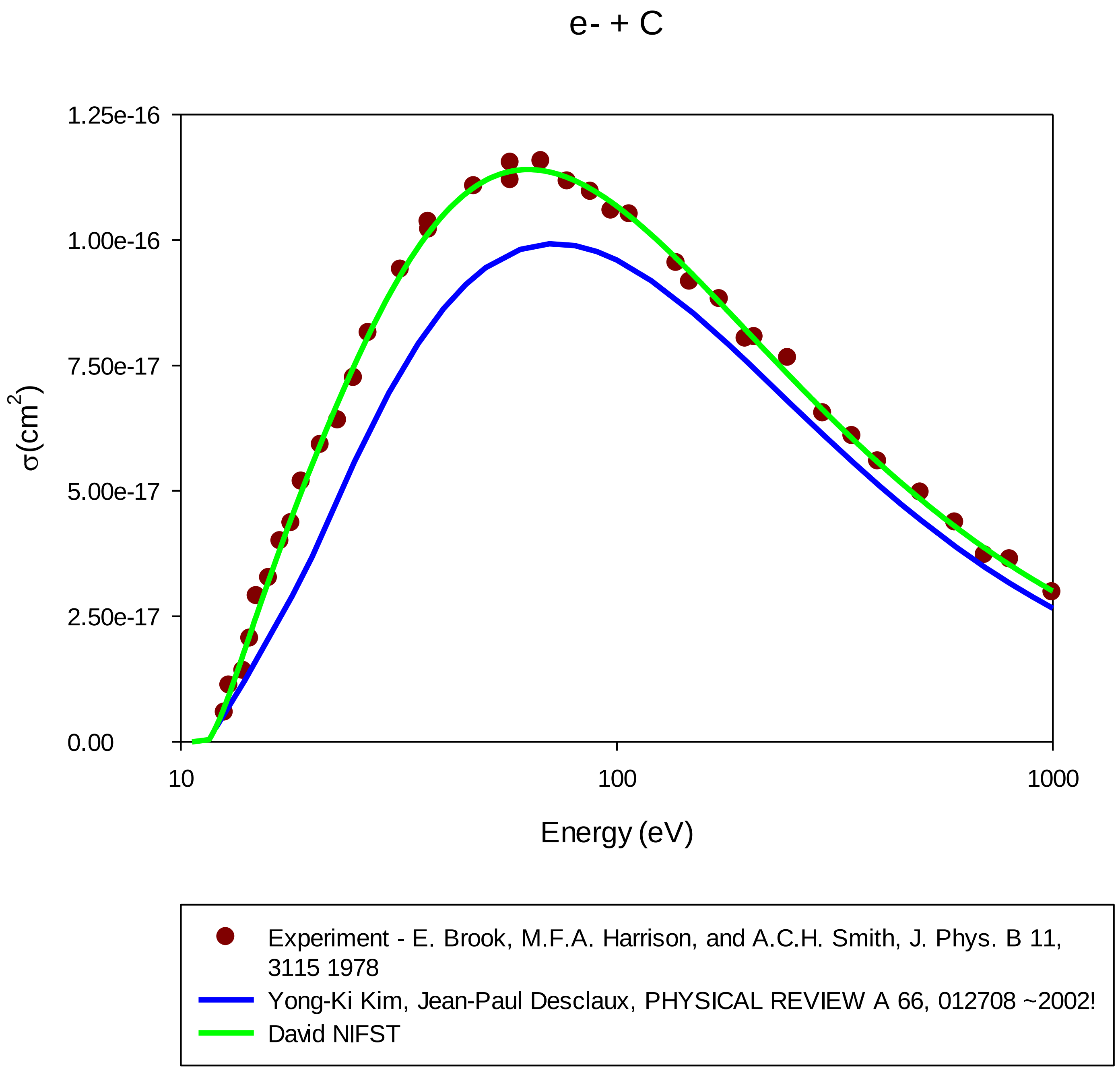

50 keV Li+ + N
1e-16
1e-17
1e-18
1e-19
0
20
40
60
80
100
Energy (eV)
dσ/dE (cm2/eV)

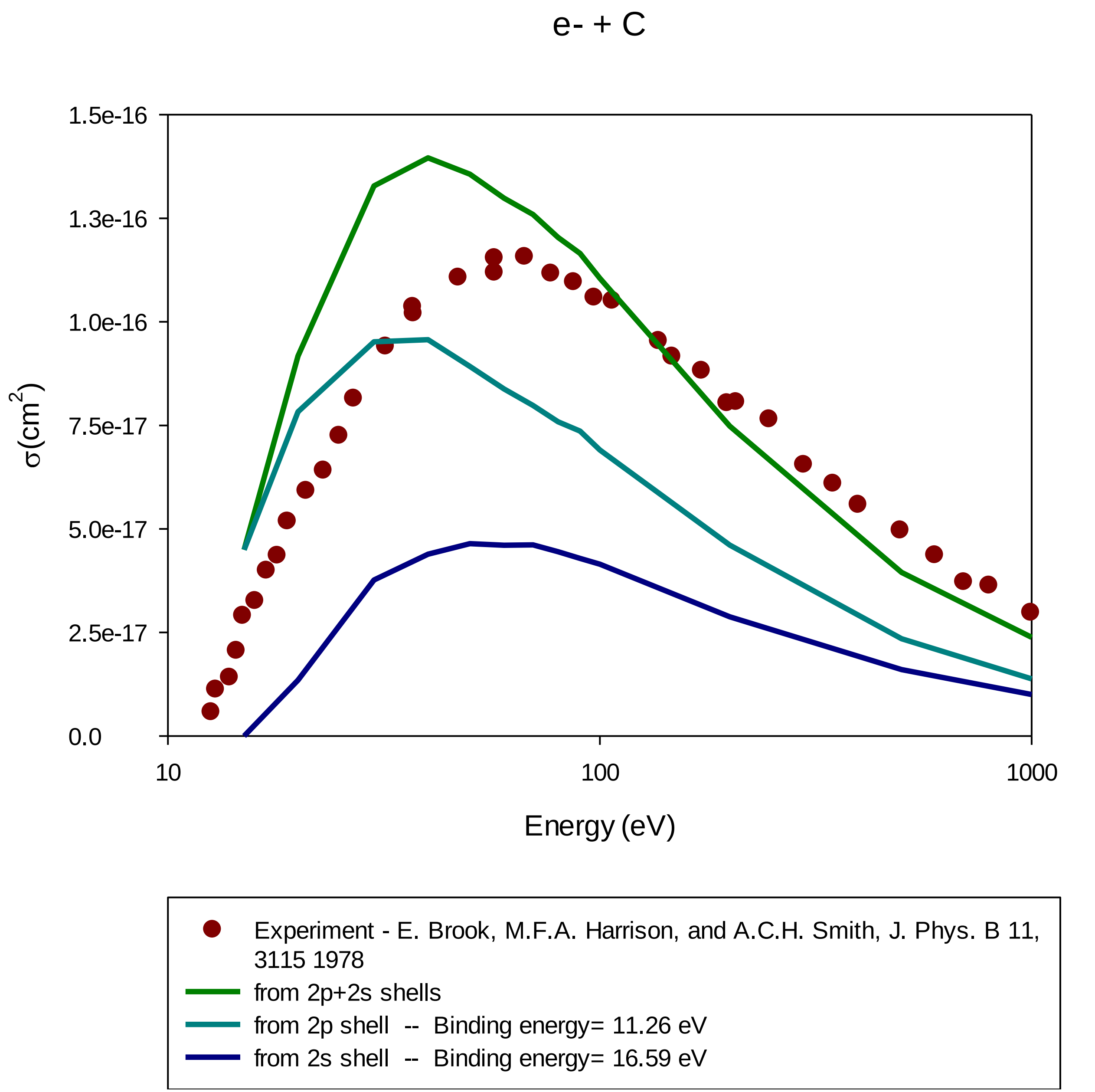
3-body simuations

e^- +C

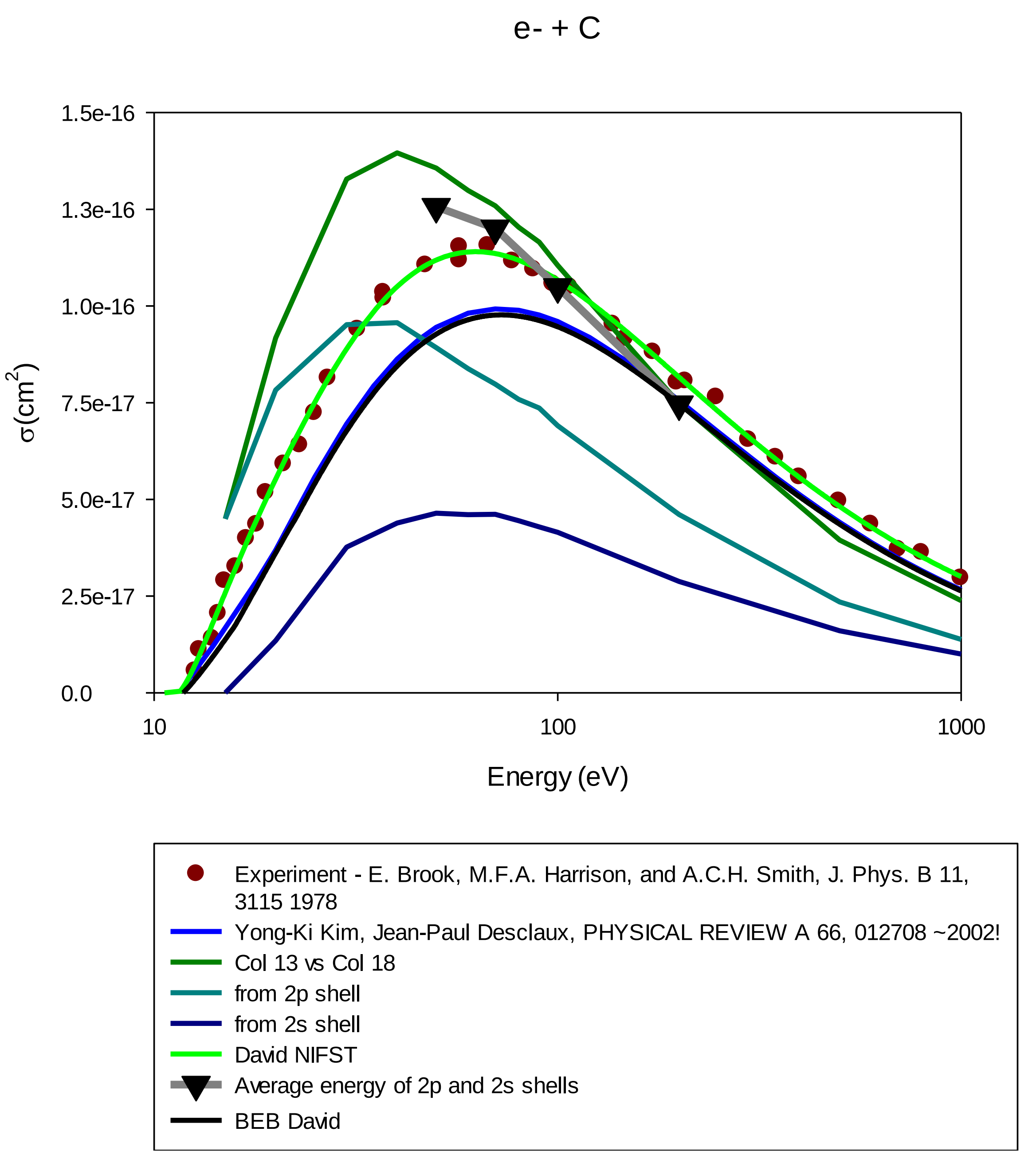


e- + C
1.25e-16
1.00e-16
7.50e-17
5.00e-17
2.50e-17
0.00
σ(cm2)
10
100
1000
Energy (eV)
Experiment - E. Brook, M.F.A. Harrison, and A.C.H. Smith, J. Phys. B 11, 3115 1978


e- + C
1.25e-16
1.00e-16
7.50e-17
5.00e-17
2.50e-17
0.00
σ(cm2)
10
100
1000
Energy (eV)
Experiment - E. Brook, M.F.A. Harrison, and A.C.H. Smith, J. Phys. B 11, 3115 1978
Yong-Ki Kim, Jean-Paul Desclaux, PHYSICAL REVIEW A 66, 012708 ~2002!
David NIFST



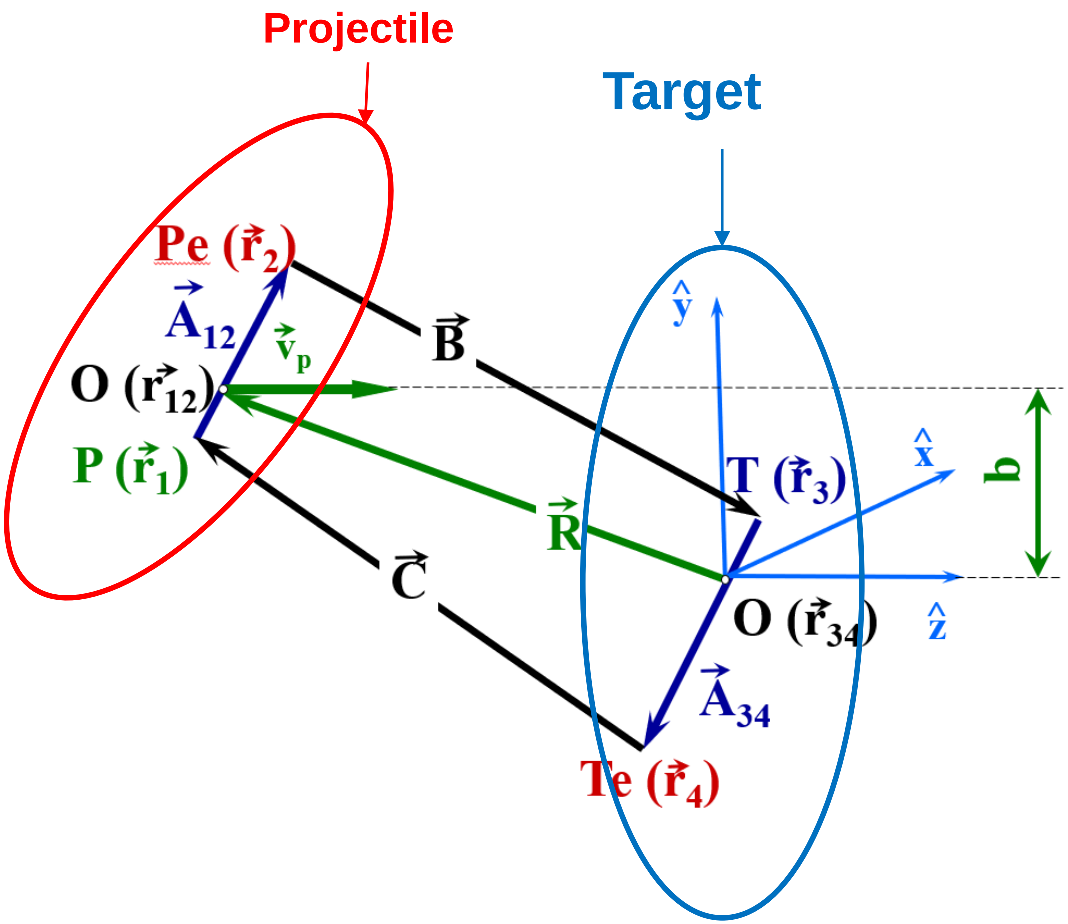
e- + C
1.5e-16
1.3e-16
1.0e-16
7.5e-17
5.0e-17
2.5e-17
0.0
σ(cm2)
10
100
1000
Energy (eV)
Experiment - E. Brook, M.F.A. Harrison, and A.C.H. Smith, J. Phys. B 11, 3115 1978
from 2p+2s shells
from 2p shell -- Binding energy= 11.26 eV
from 2s shell -- Binding energy= 16.59 eV



e- + C
1.5e-16
1.3e-16
1.0e-16
7.5e-17
5.0e-17
2.5e-17
0.0
σ(cm2)
10
100
1000
Energy (eV)
Experiment - E. Brook, M.F.A. Harrison, and A.C.H. Smith, J. Phys. B 11, 3115 1978
Yong-Ki Kim, Jean-Paul Desclaux, PHYSICAL REVIEW A 66, 012708 ~2002!
Col 13 vs Col 18
from 2p shell
from 2s shell
David NIFST
Average energy of 2p and 2s shells
BEB David

4-body simuations

4-body CTMC approach



$$m_i \frac{d^2 \overrightarrow{r_i}}{dt^2} = \sum_j \frac{z_i z_j (\overrightarrow{r_i} - \overrightarrow{r_j})}{|\overrightarrow{r_i} - \overrightarrow{r_j}|^3} \qquad \begin{array}{r} i, j = 1, 2, 3, 4 \\ j \neq i \end{array}$$

Classical exit channels

$$X + H_2 \rightarrow X^+ + H_2 + e_p$$
$$X + H_2 \rightarrow X^+ + H_2 + e_t$$
$$X + H_2 \rightarrow X^+ + H_2^+ + 2e$$
$$X + H_2 \rightarrow X^+ + H_2^-$$
$$X + H_2 \rightarrow X^- + H_2^+$$

```
                              Li -> H2

                    I D E N T I F I E R =  eccmel

     Pm=  0.1285D+05       Em=  0.1000D+01      Tm=  0.3673D+04    em=  0.1000D+01
     Pz=  0.1300D+01       Ez= -0.1000D+01      Tz=  0.1165D+01    ez= -0.1000D+01
  Ubind=  0.56700000D+00  Rstart=  0.50000000D+02  Rstop=  0.10000000D+03
 Ubind2=  0.19807438D+00   Bmin=  0.00000000D+00    Bmax=  0.10000000D+02
   V(TE) : coulomb        V(PE) : coulomb        V(TP) : coulomb
   V(Te) : coulomb        V(Pe) : coulomb        V(Ee) : coulomb
          Vp=  0.8947D+00 au.     Ep=  0.1400D+03 KeV

      ntotal current=   100000     ntotal expected=   100000

              direct=    77752              äbiei=  0.45768185D+06
   target ionization=     4022              äbiei=  0.52556876D+04
      projectile ion=     3524              äbiei=  0.10896574D+05       0
 exchange & rearran.=     2160              äbiei=  0.39615015D+04
      capture to pro=     2954              äbiei=  0.47227921D+04
   capture to target=      439              äbiei=  0.15209685D+04
    target&pro. ion.=      708              äbiei=  0.95301327D+03
    targetion & cap.=     2024              äbiei=  0.59007563D+04
    pro. ion & cap. =     6417              äbiei=  0.95129487D+04
      anomal trajec.=        0              äbiei=  0.00000000D+00
```

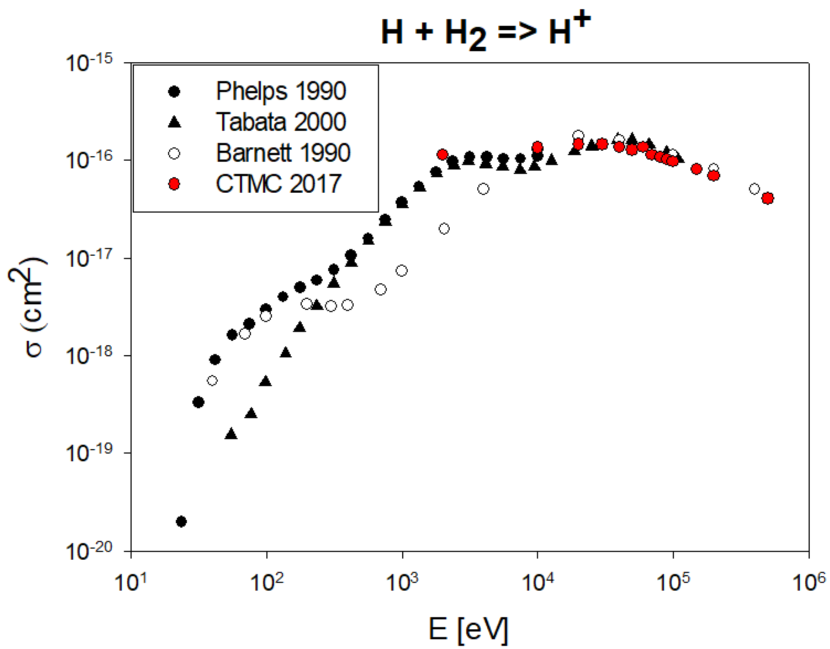
$H + H_2$

H

- $m_1 = 1{,}836*10\text{^}3\ m_e\ ,\ m_2 = m_e$
- $z_1 = -\ 1(-z_e\ ),\ z_2 = z_e$
- $E_{12} = -\ 0{,}5\ u$

H_2

- $m_3 = 3{,}673*10\text{^}3\ m_e,\ m_4 = m_e$
- $z_3 = 1{,}165(-z_e\ ),\ z_4 = z_e$
- $E_{34} = 0{,}567\ u$



V. Phelps - Cross Sections and Swarm Coecients for H + , H2 + , H3 + , H, H2, and H- in H2 for Energies from 0.1 eV to 10 keV

T. Tabata, T. Shirai - ANALYTIC CROSS SECTIONS FOR COLLISIONS OF H+, H+2 , H+3 , H, H2, AND H< WITH HYDROGEN MOLECULES

F. Barnett, J. A. Ray, E. Ricci, M. I. Wilker, W. W. Mc-Daniel, E. W. Thomas, and H. B. Gilbody, Atomic Data for Controlled Fusion Research,"Report ORNL- 5206, Vol. 1, Oak Ridge National Laboratory

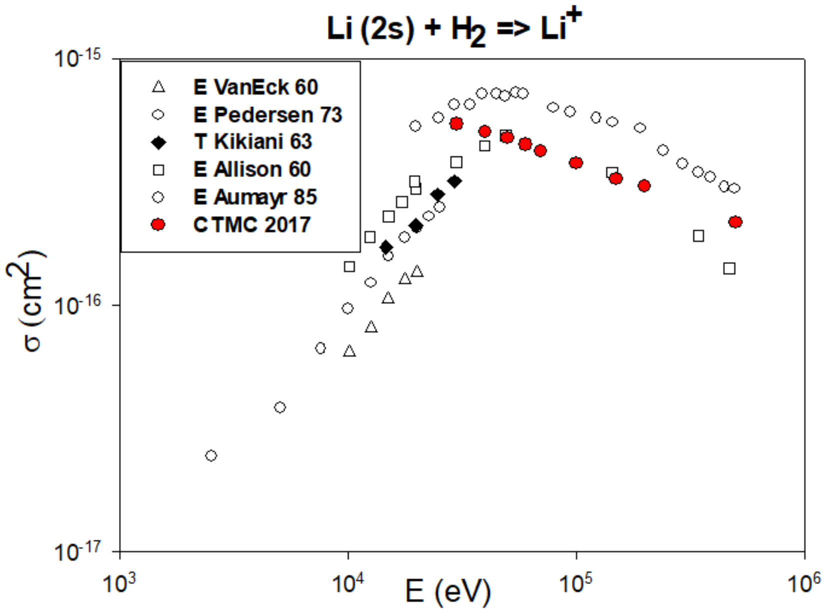
Li + H_2

Li

- $m_1 = 1{,}2852*10\text{^}4\ m_e\ ,\ m_2 = m_e$
- $z_1 = 1{,}3(-z_e),\ z_2 = z_e$
- $E_{12} = 0{,}19807438\ u$

H_2

- $m_3 = 3{,}673*10\text{^}3\ m_e,\ m_4 = m_e$
- $z_3 = 1{,}165(-z_e),\ z_4 = z_e$
- $E_{34} = 0{,}567\ u$



Plan -- Outlook

Classical simulations

in charged particles-atom collsions

- **Ionization**
- **State Selective Exciation**
- **State Selective Charge Transfer**

Conclusions

- Classical method (CTMC) reproduce different experiments for collisions between charged particles and atoms,
- gives accurate cross sections for ionization

  Capture

  Excitation
- valid in wide projectile energy range
- can descibe partial cross sections

Thanks for your attention!