Data for Modeling of Positron Collisions and Transport in Gases

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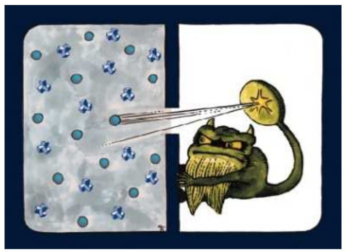
Thanks to M Brunger, J Marler, C Surko, M Charlton, R Campeanu, G Garcia R. White, M Suvakov, R McEchran, C Makochekanwa, D Van Der Werf,

…



LABORATORY FOR GASEOUS ELECTRONICS
INSTITUTE OF PHYSICS BELGRADE

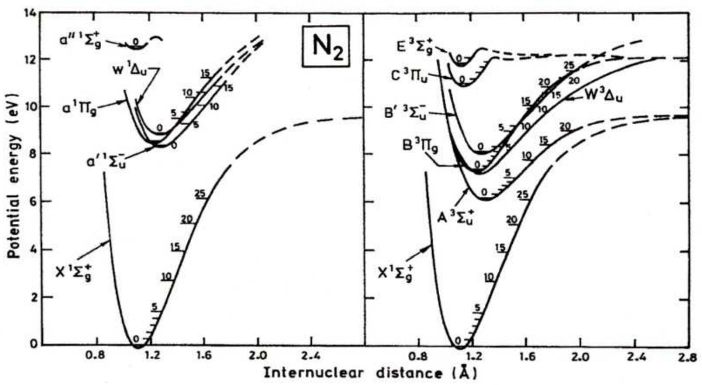
ARC Centre of Excellence for Antimatter-Matter Studies

THE AUSTRALIAN NATIONAL UNIVERSITY

Motivation & Background

- Positrons are interesting
  - different Coulomb interactions (cf electrons)
  - different spectroscopy
  - Positronium formation
  - Experiments with antimatter

singlets triplets



- Positrons are useful -applicable
  - biomedical science
    - PET diagnostic
    - positherapy
  - materials science
    - nanoscale probe of “open space” and defects in materials
  - Modeling of traps=production of antimatter
    - Generating antihydrogen relies on gas filled traps

- .

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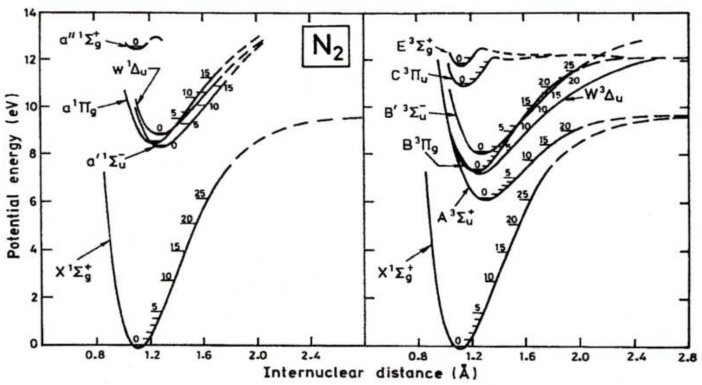

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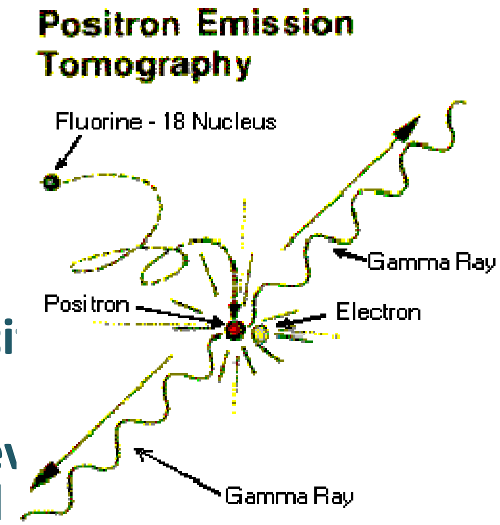
    - Generating antihydrogen relies on gas filled traps

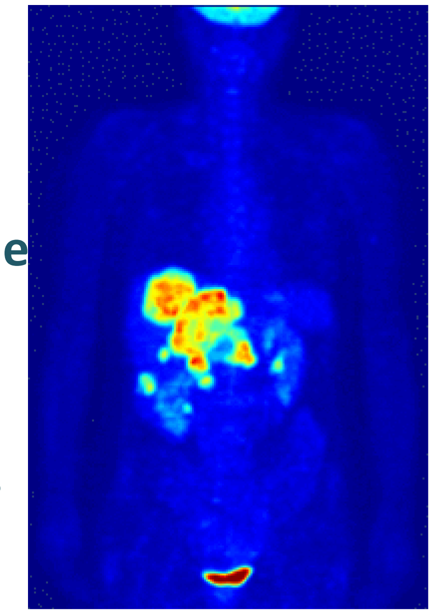
- publishable

Cross sections should be collected? Why?



- **Application of data in dose adjustment**
  - **Semi empirical data used**
  - **More accurate and scietntifically based predictions**
  - **Extension to new systems, complex systems, some speci channels for specific processes, ….**
  - **Average properties like energy deposition need to be rev as primary damage stems from very localized individual events**

- **Can cross sections be exploited ?**
  - **CAN WE USE THE MEASURED BINARY COLLISION CROSS SECTIONS IN MODELING OF POSITRONS (THUS MAKING THEIR CROSS SECTIONS WORTHY OF COMPILATIONS)**
  - **Is it possible to develop swarm experiments to normalize the sets**
  - **Is it possible to develop benchmarks and experimental benchmarks**
  - **how to translate binary collision data to collisions in liquids and solids !!!!**



1st step – trap and thermalize positrons

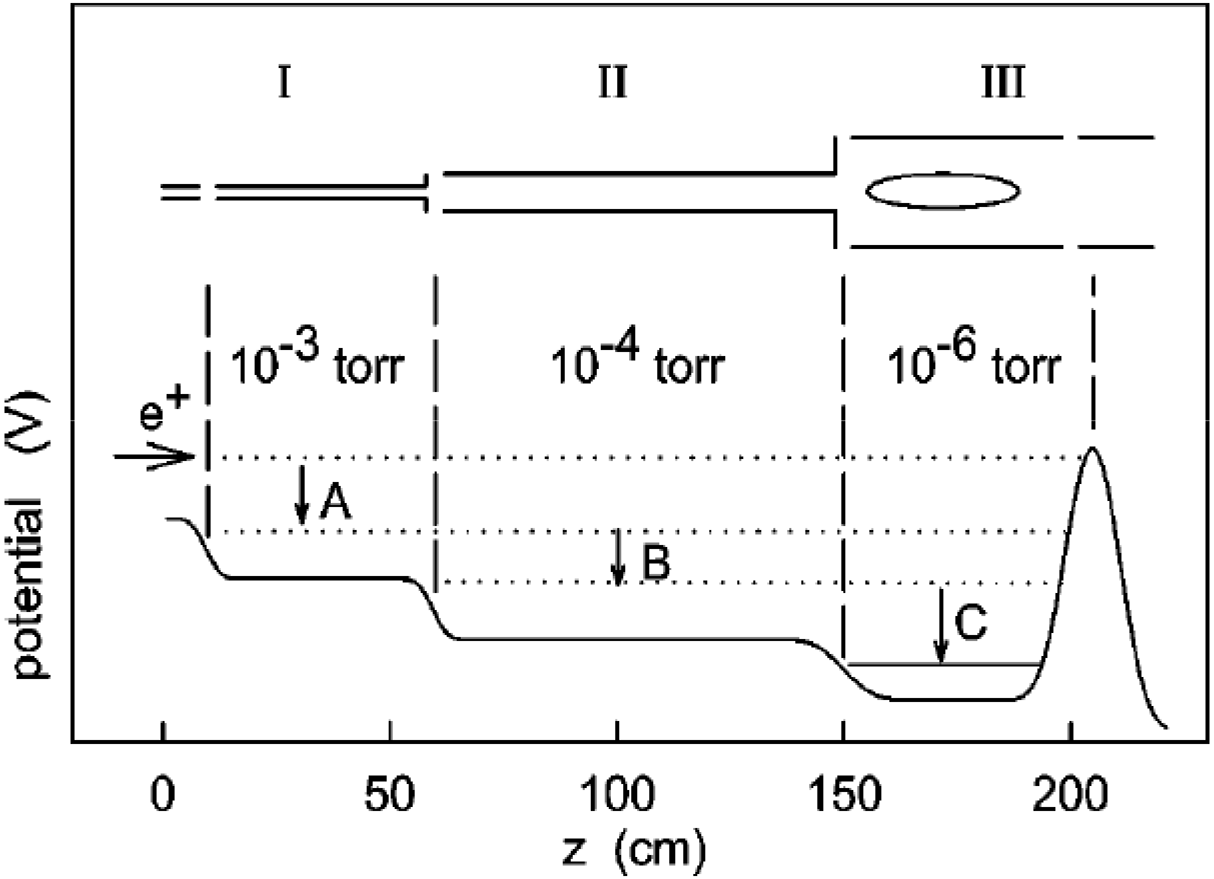
2nd step – measure positron molecule cross sections

- Gas filled traps
- Penning Malmberg Surko
- Crossed beam or beam /cell experiments
- Swarms

3rd step – generate a complete set

4th step – model application

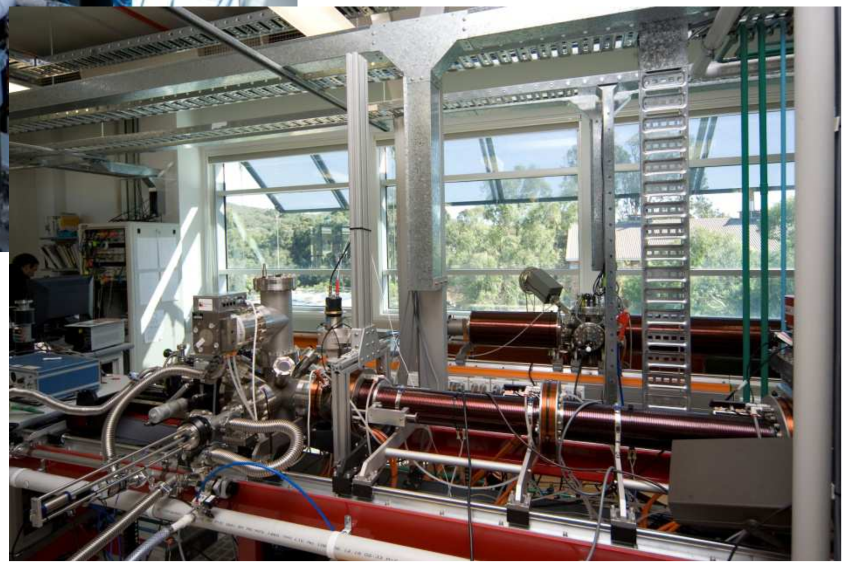
Penning Malmberg Surko trap



- N_2 , H_2 , CO , CO_2 , CF_4

C. M. Surko and R. G. Greaves, **Phys. Plasmas 11**, 2333 (2004)

CAMS experiment



New sources of data- gas filled traps
Surko Laricchia Charlton Zecca
CAMS ANU- SJ Buckman J Sullivan

How do we model ionized gases -swarms

- Number balance
- Momentum balance
- Energy balance

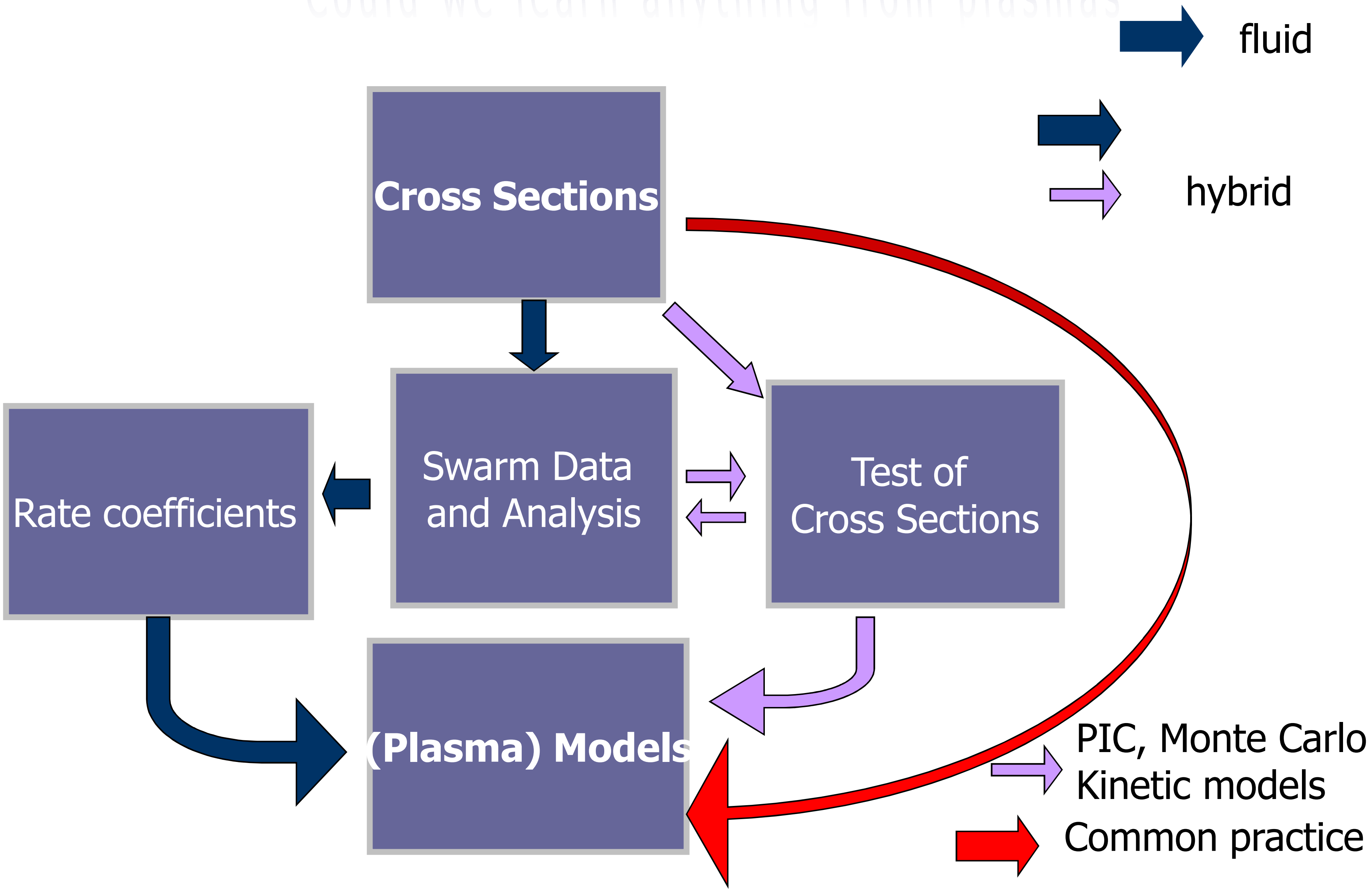
- Complete set of cross sections

- Individual cross sections not sufficient

- Basic tools: solutions to Boltzmann equation, Monte Carlo simulations, very accurate experiments, transport data and rate coefficients

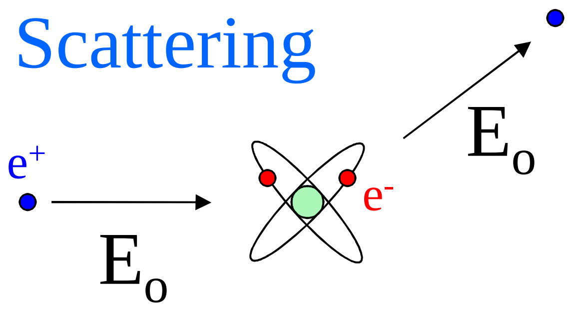
how do we use atomic and molecular collision data in modeling

Could we learn anything from plasmas

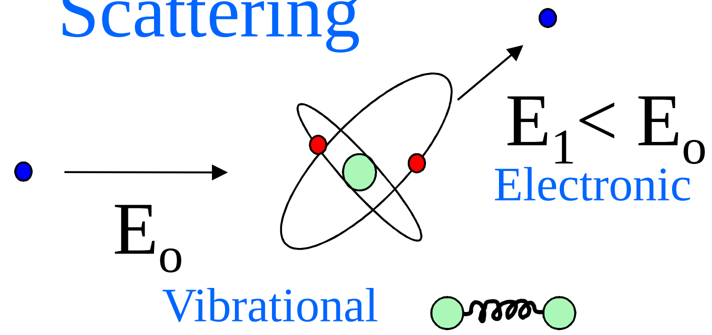


Positron-matter interactions: Cross sections

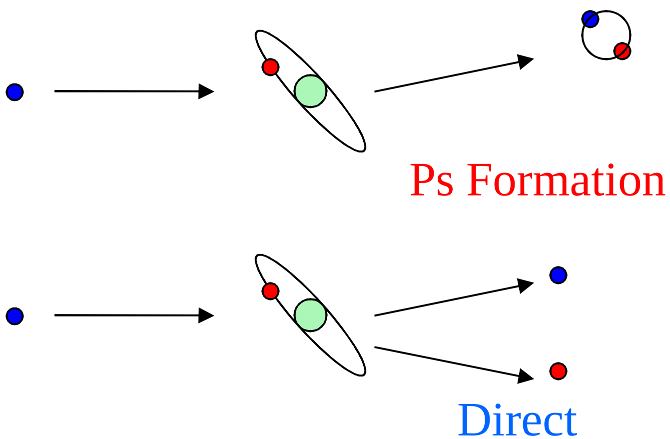
Elastic Scattering



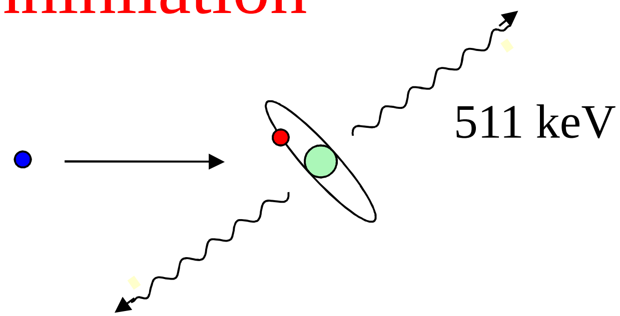
Inelastic Scattering



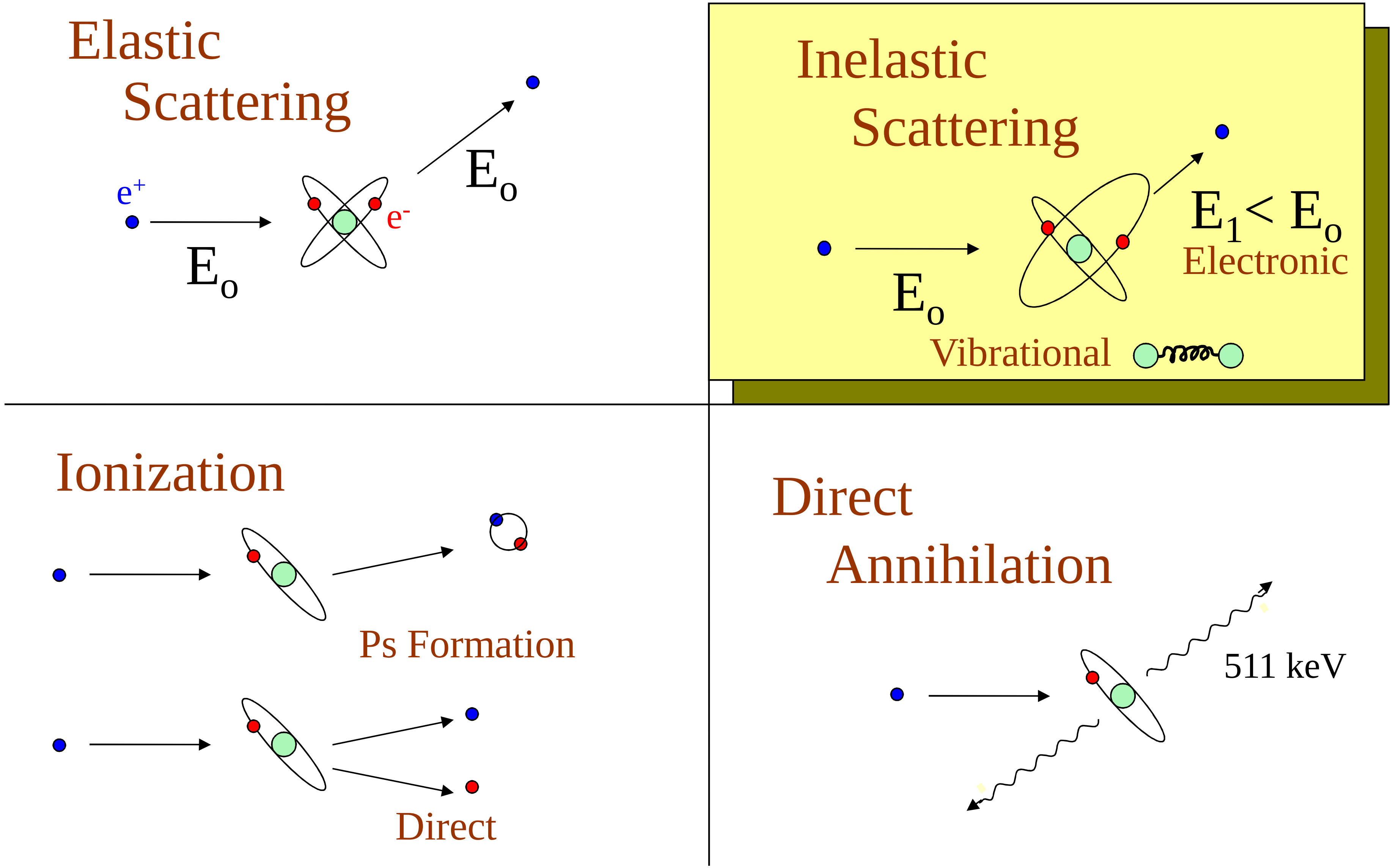
Ionization



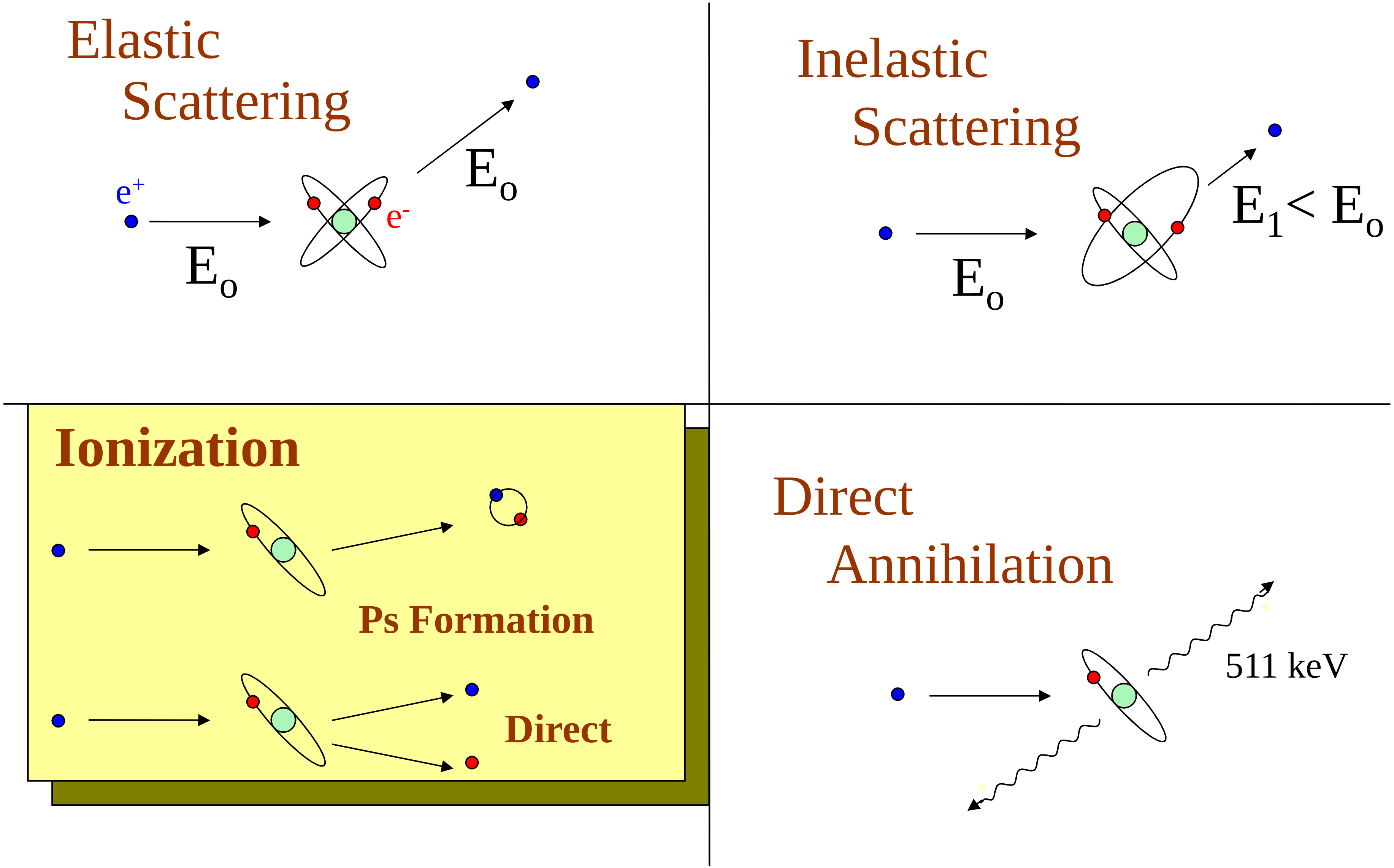
Direct Annihilation



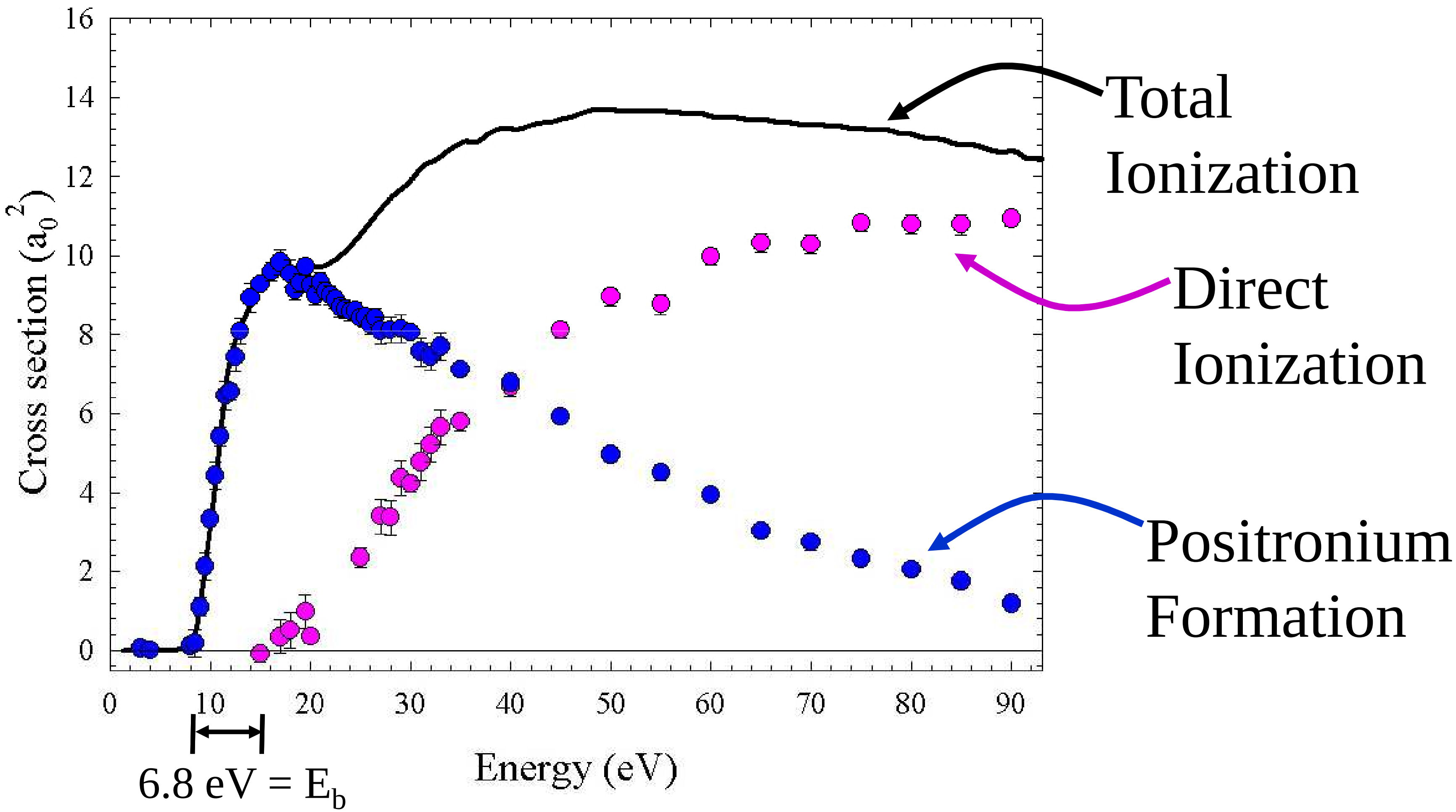
Positron-matter interactions



Positron-matter interactions

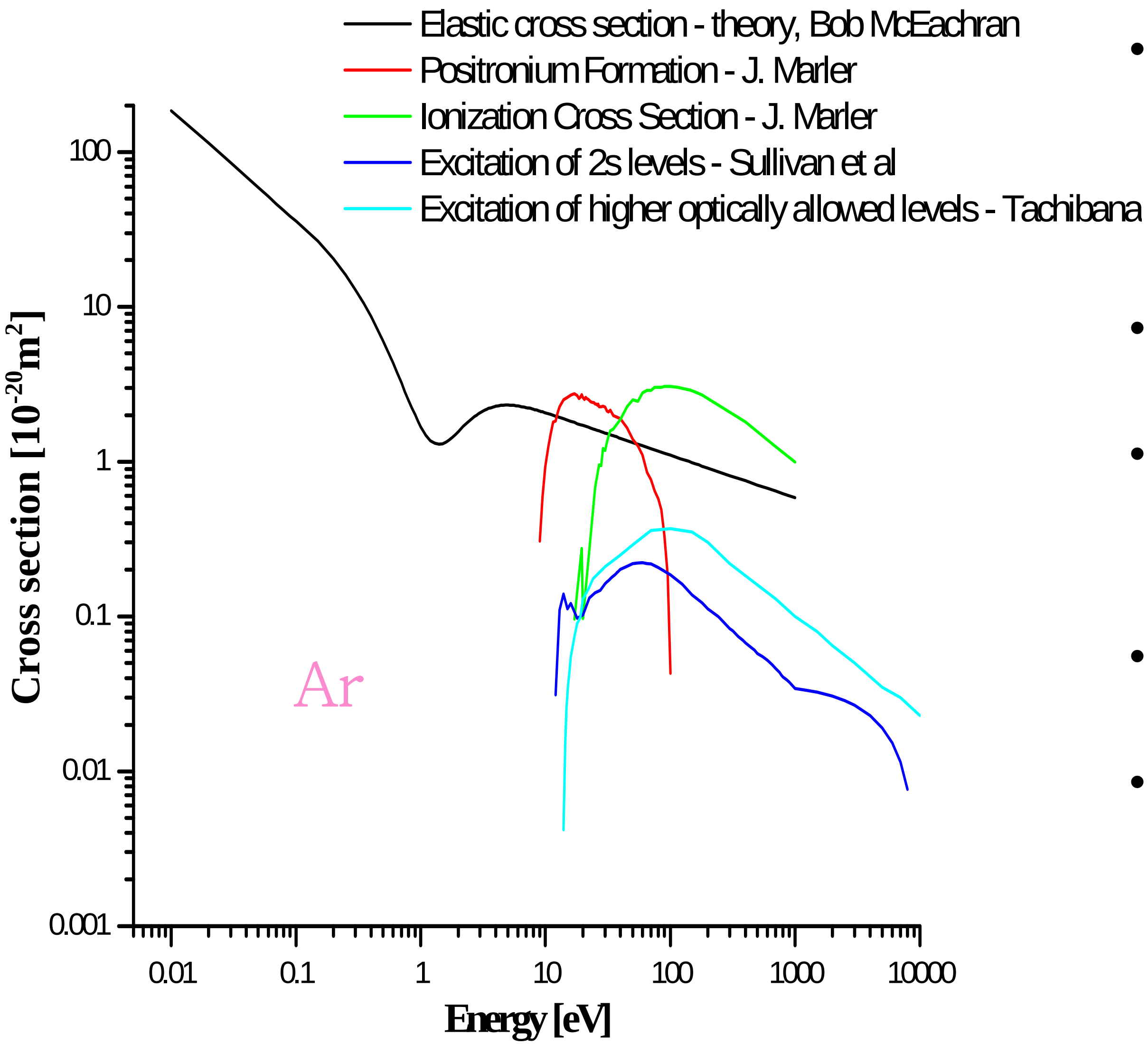


Ionization of Argon



UCSD, Marler et al., Phys Rev A (2005)

ARGON
a complete set of cross sections



- **Total cross sections were measured by Kauppila and coworkers [1] and total elastic cross sections were calculated by McEchran [2]: theoretical data allowed us to separate elastic and inelastic processes.**
- **We have extrapolated the theoretical results to low and high energies.**
- **The positronium formation and ionization were taken from Marler et al [3] while direct annihilation has been neglected.**
- **Measured excitation cross sections for the lowest states of argon were used [4].**
- **We have also added the cross section for higher singlet levels for electron excitation [5] of argon.**

Ar

total:

[a1] W. E. Kauppila and T. S. Stein, Adv. At., Mol., Opt. Phys. 26, (1990) 1]

[a2] McEchran [personal communication].

Ps.formation and ionization

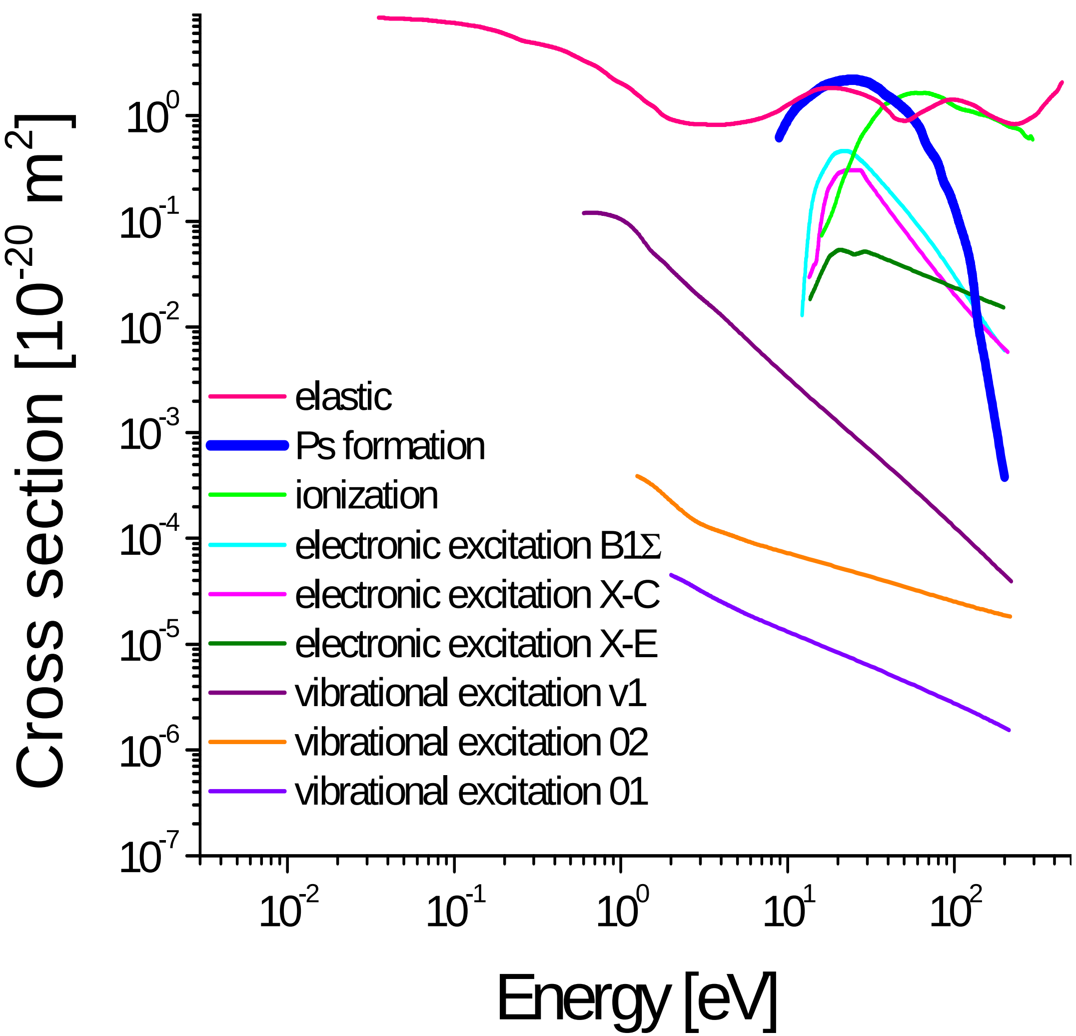
[a3] J. P. Marler, J. P. Sullivan, and C. M. Surko, Phys. Rev. A 71, (2005) 022701

Electronic excitation:

[a4] J. P. Sullivan, J. P. Marler, S. J. Gilbert, S. J. Buckman and C. M. Surko Phys. Rev. Lett. 87 073201 (2001).

[a5] A.V. Phelps and K. Tachibana personal communication (1985)- higher singlet states for e-Ar

HYDROGEN
a complete set of cross sections



- Total elastic cross sections were measured by Hoffman *et al.* [c1]
- Cross sections for electron excitations X-E and X-C were taken from Arretche and Lima [c2] and for X-B from Sullivan et al. [c3]
- The positronium formation and ionization were taken from Fromme *et al*. [c4]
- Vibrational cross section for v1 mode was taken from Sullivan et al. [c5] and for 0-2 and 0-3 from Gianturco and Mukherjee [c6]
- Rotational excitation the same as for electrons [c7]

H_2

total: [c1] K. R. Hoffman, M. S. Dababneh, Y. F. Hsieh, W. E. Kauppila, V. Pol, J. H. Smart, T. S. Stein, *Phys. Rev*. **A25** (1982) 1393-1403

Electronic excitation: X-A and

X-C [c2] F. Arretche, M. A. P. Lima, *Phys. Rev*. **A74** (2006) 042713

X-B [c3] J. P. Sullivan, J. P. Marler, S.J. Gilbert, S.J. Buckman, C. M. Surko, *Phys. Rev. Lett*. **87** (2001) 073201

Ps.formation

[c4] D. Fromme, G. Kruse, W. Raith, G. Sinapius, *J. Phys. 8: At. Mol. Opt. Phys. 21* (1988) L261-L265

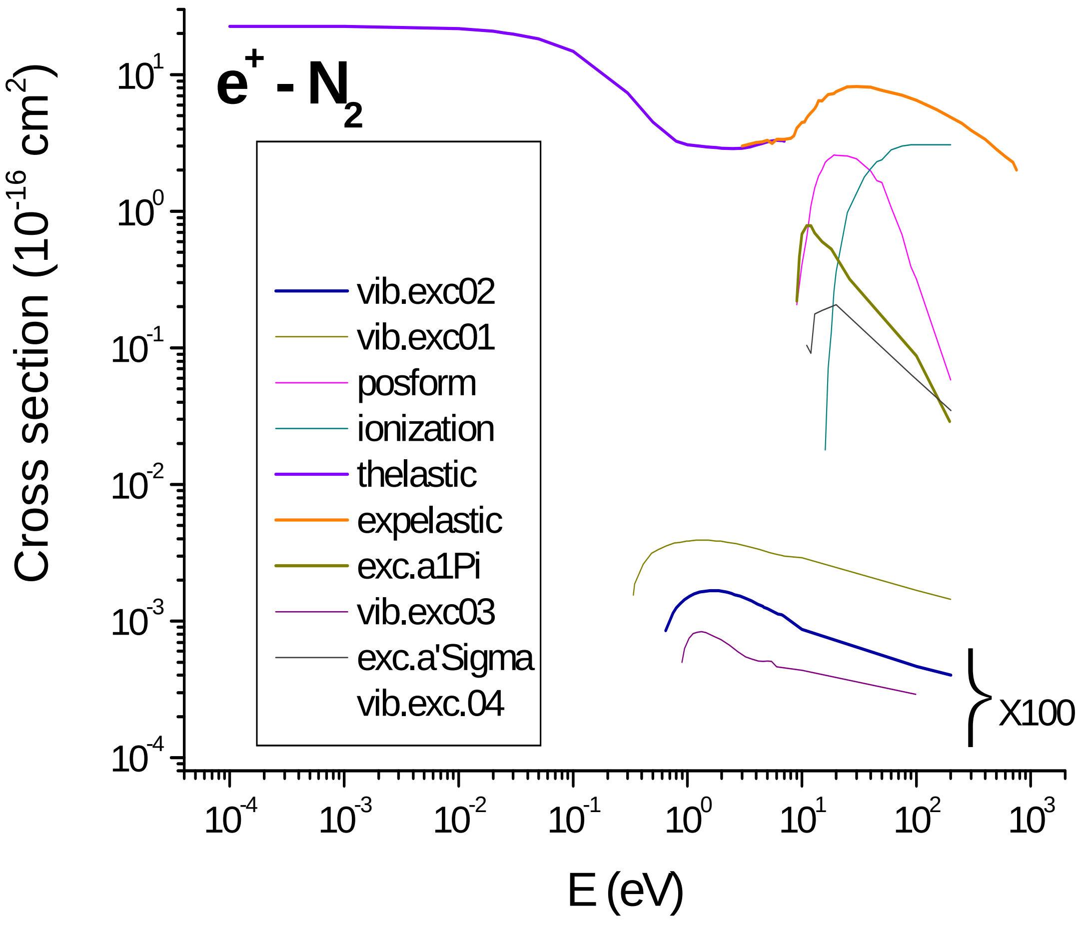
Vibrational excitation

0-1 [c5] J. P. Sullivan, S. J. Gilbert, C. M. Surko, *Phys. Rev. Lett*. **86** (2001) 1494

0-2 0-3 [c6] Gianturco Mukharje

Rotational excitation: just like electrons??? [c7] ANU data

NITROGEN
a complete set of cross sections



- Total cross sections were measured by Hoffman *et al*. [b1] and total elastic cross sections were calculated by de Carvalho *et al*. [b2].
- The positronium formation and ionization were taken from Marler and Surko [b3], while direct annihilation has been neglected.
- Added the cross sections for electron excitations [b4]
- Vibrational cross sections were taken from Gianturco and Mukherjee [b5]
- Rotations Gerjoy Stein for electrons

N_2

total:

[b1] K. R. Hoffman, M. S. Dababneh, Y. F. Hsieh, W. E. Kauppila, V. Pol, J. H. Smart, T. S. Stein, *Phys. Rev*. **A25** (1982) 1393-1403

[b2] C. R. C. de Carvalho, T. Marcio, do N. Varella, M. A. P. Lima, E. P. da Silva, J. S. E. Germano, *Nucl. Instrum. And Methods in Phys. Res*. **B171** (2000) 33-46

Ps.formation

[b3] J. P. Marler, C. M. Surko, *Phys. Rev*. **A72** (2005) 062713

Electronic excitation:

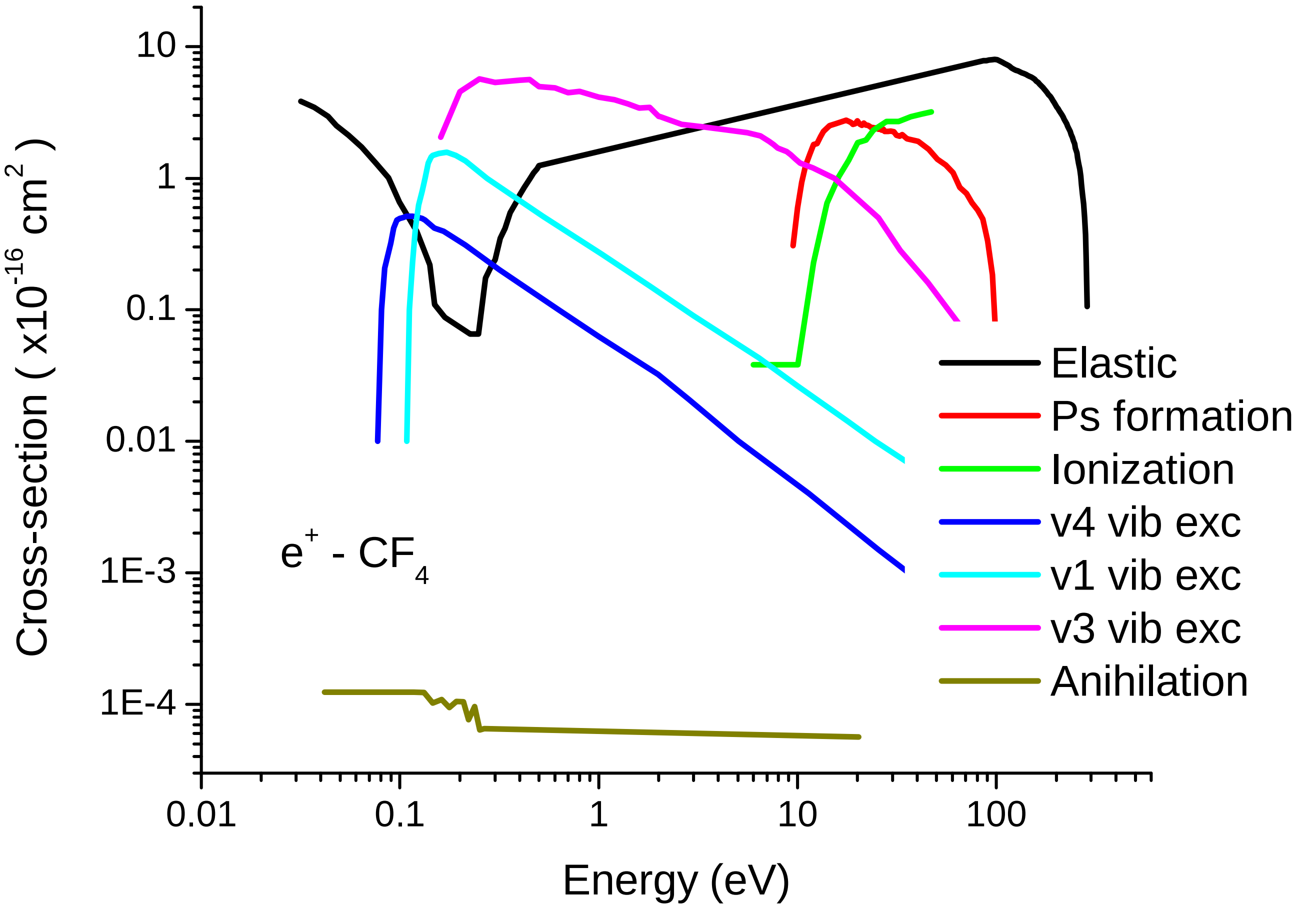
[b4] J. P. Marler, C. M. Surko, Phys. Rev. A 72 (2005) 062713.

Vibrational excitation

- [b5] F. A. Gianturco, T. Mukherjee, Phys. Rev. A 55 (1997)1044–1055.J. P. Sullivan, private communication (2007).

Rotational excitation: Gerjoy Stein formulas- non-resonant

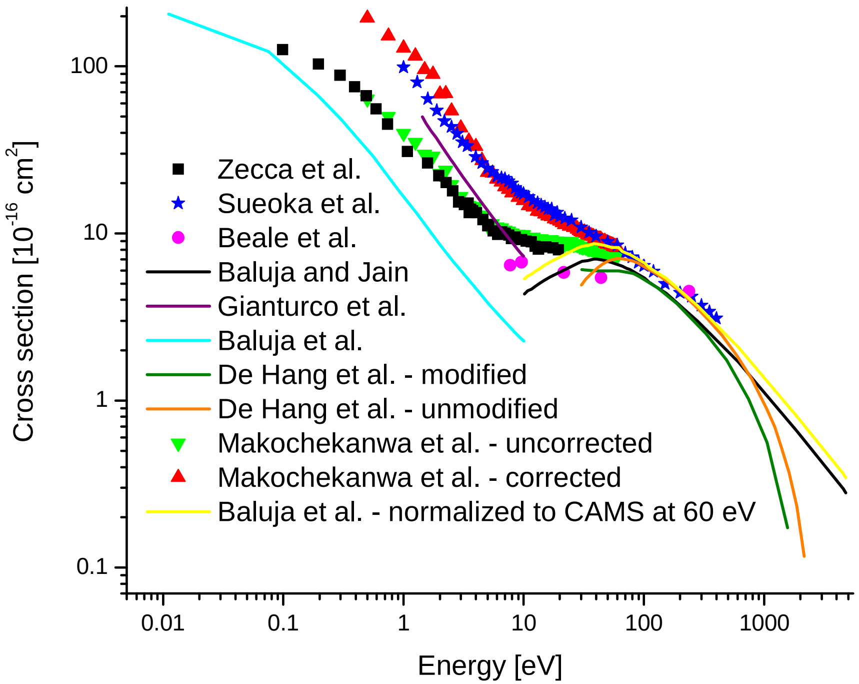
CF_4 set of cross sections



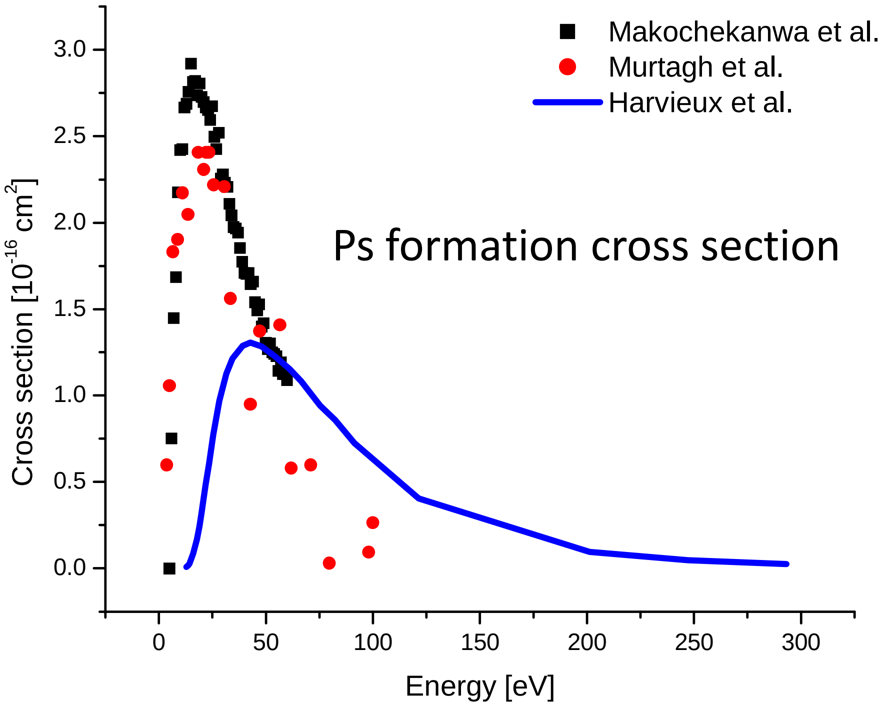
Cross sections for electronic excitations are missing! They are not available in the literature!

WATER VAPOUR
a complete set of cross sections

Total cross section



Ps formation cross section



our contribution to collision and transport database

electrons:

- H_2, D_2, CO, SF_6, Ar, SiH_4, Si_2H_6, CF_4, NO, N_2O, $C_2H_2F_4$, HBr, ...

ions:

- Ne^+, F^-, Cl^-, CF_3^-, O^-, SF_6^-

positrons:

- Ar, H_2, N_2, H_2O, CF_4

transport data:

- drift velocities
- mean energies
- characteristic energies
- diffusion coefficients
- ionization coefficients
- rate coefficients
- distribution functions

DC: E, EXB fields

AC: E, EXB fields

http://mail.ipb.ac.rs/~cep/ipb-cnp/ionsweb/database.htm

Positron transport in gases:
The ultimate non-conservative transport

Transport coefficients
Monte Carlo simulations

drift velocity

$$w_i = \frac{d}{dt}\langle x_i \rangle$$ **Bulk**

$$W_F = \langle \vec{v} \rangle$$ **Flux**

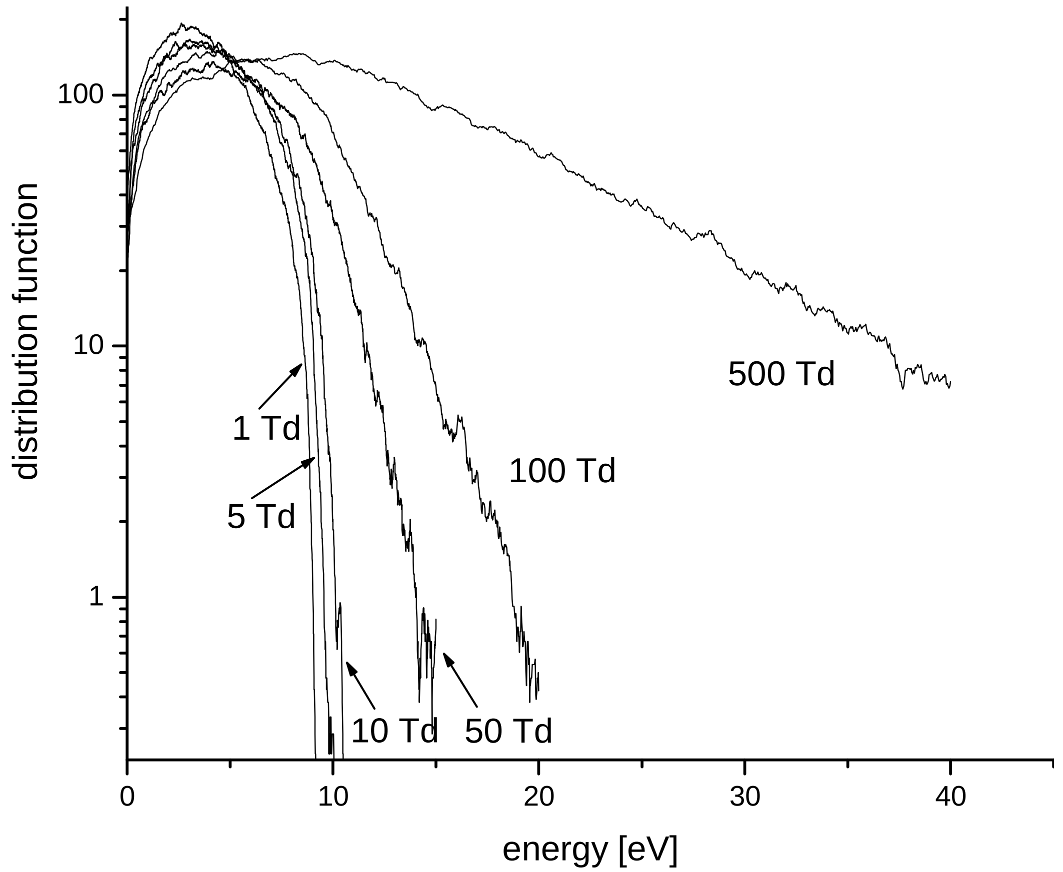
diffusion tensor

$$D_{Bxx} = \frac{1}{2}\frac{d}{dt}\left(\langle x^2 \rangle - \langle x \rangle^2\right)$$

$$D_{Fxx} = \langle x v_x \rangle - \langle x \rangle \langle v_x \rangle$$

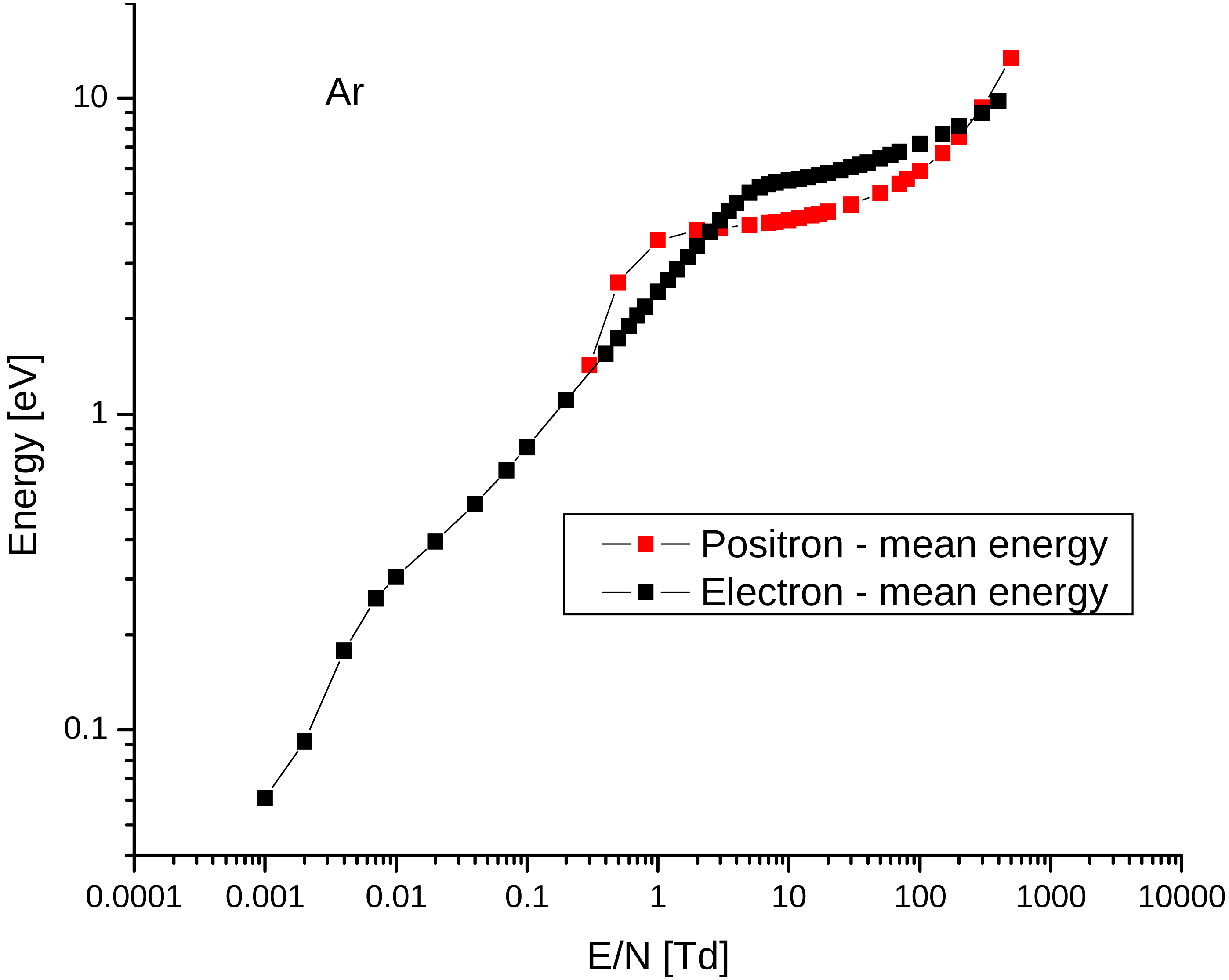
$$W \approx w - \frac{2\langle\epsilon\rangle}{3e}\frac{d\langle\nu_a(\epsilon)\rangle}{dE} \approx w - \frac{2\langle\epsilon\rangle}{3e}\frac{d\nu_a(\langle\epsilon\rangle)}{d\langle\epsilon\rangle}\frac{d\langle\epsilon\rangle}{dE}$$

Argon: a case study?!



Positrons in argon

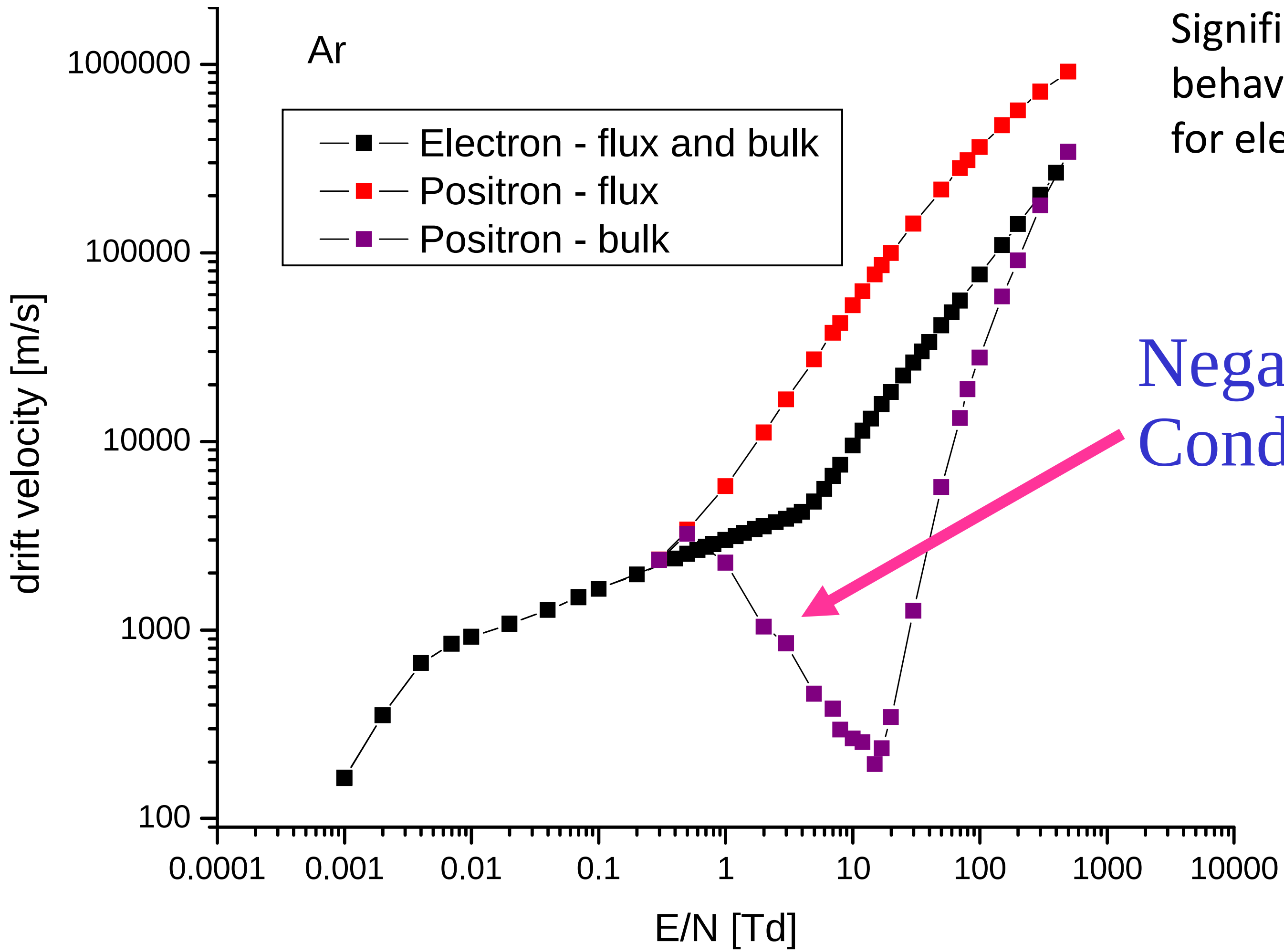
Argon: Electrons and Positrons Mean Energies



Slightly different E/N dependence for the mean energies for electrons and positrons

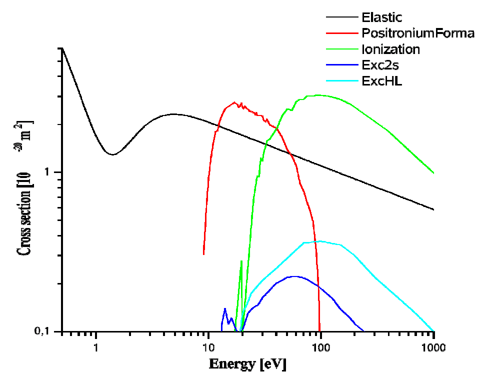
Example: (e+,Ar) NDC for *W* (not *w**)

Monte-Carlo



Significantly different behavior of drift velocities for electrons and positrons!

Negative differential Conductivity - NDC



"R" = Ps formation

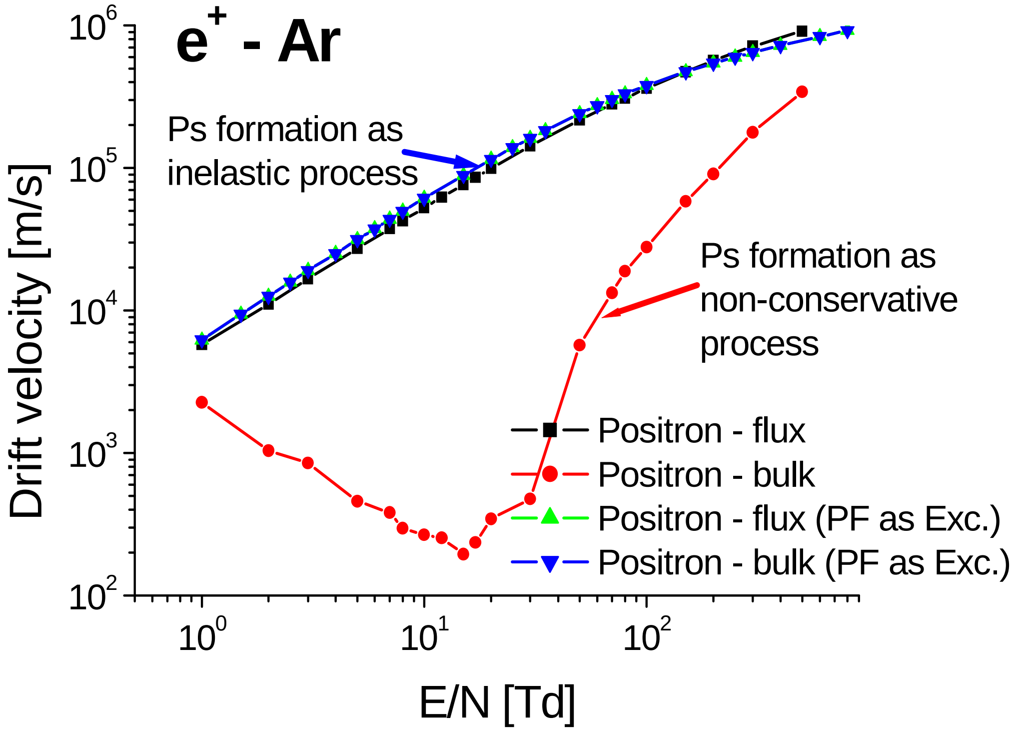
$\nu'_R > 0$, $W < w^*$, 'attachment' cooling

$$W \approx w - \frac{2\langle\epsilon\rangle}{3e}\frac{d\langle\nu_a(\epsilon)\rangle}{dE} \approx w - \frac{2\langle\epsilon\rangle}{3e}\frac{d\nu_a(\langle\epsilon\rangle)}{d\langle\epsilon\rangle}\frac{d\langle\epsilon\rangle}{dE}$$

What is NDC?

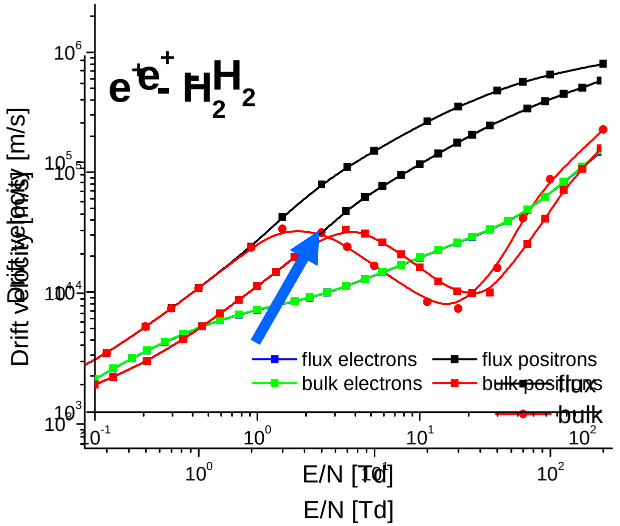
NDC – decrease of the drift speed with increasing driving field

- What is the nature of the NDC?
- Electrons vs positrons
- Non-conservative processes
- What is the role of non-conservative processes?



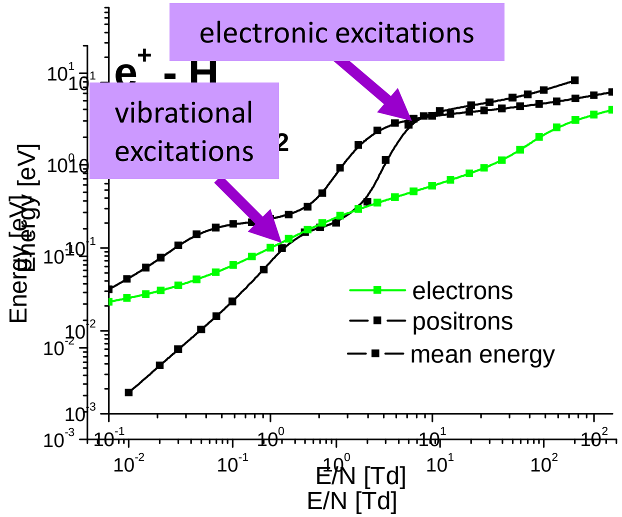
Z. Lj. Petrovic, R. W. Crompton, G. N. Haddad, Aust. J. Phys. 37 (1984) 23-24
R. E. Robson, Aust. J. Phys. 37 (1984) 35
R. Robson, J. Chem. Phys. 85 (1986) 4486
S. B. Vrhovac, Z.Lj. Petrovic, Phys. Rev. E 53 (1996) 4012

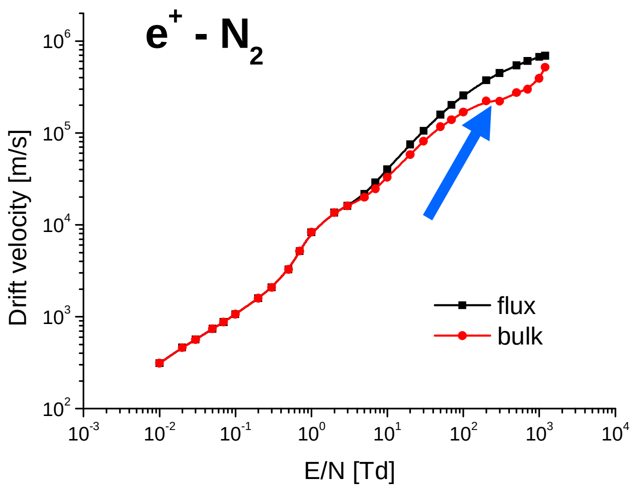
Example – H_2 and N_2



The difference between electron and positron's transport properties.

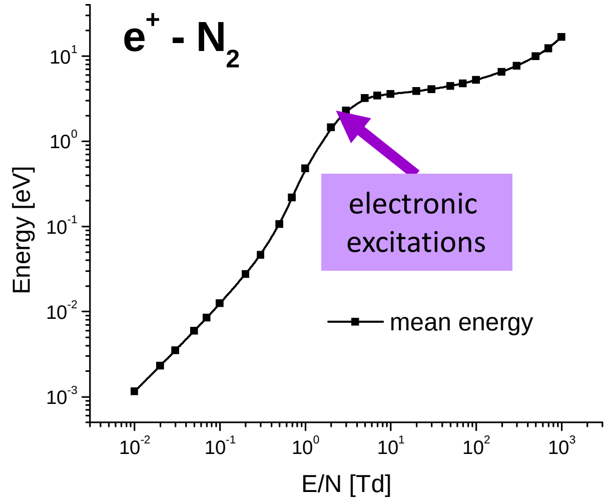
There is no NDC for positrons in N_2!!!





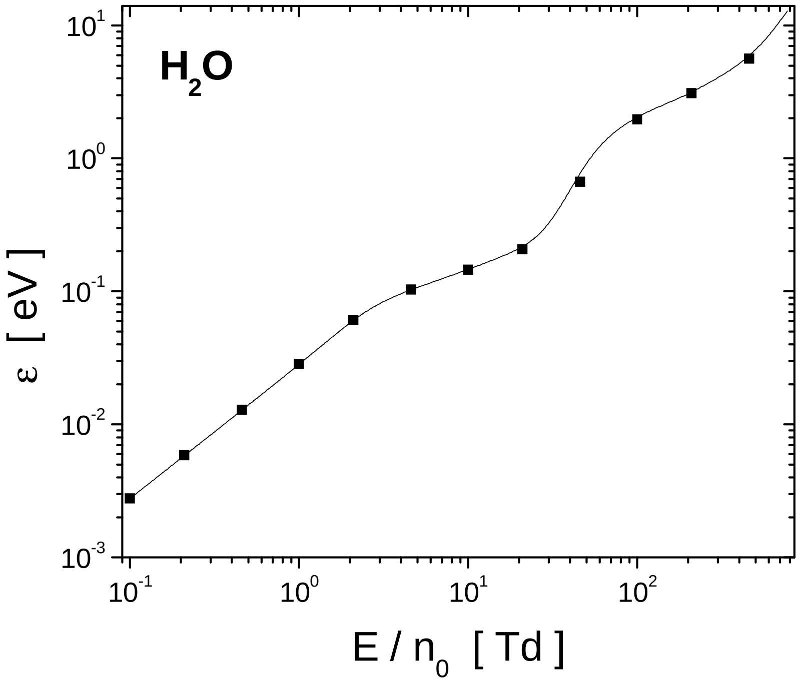
The explanation is hidden in cross sections.

Shape of mean energy dependence on E/N can reveal more about cross sections!

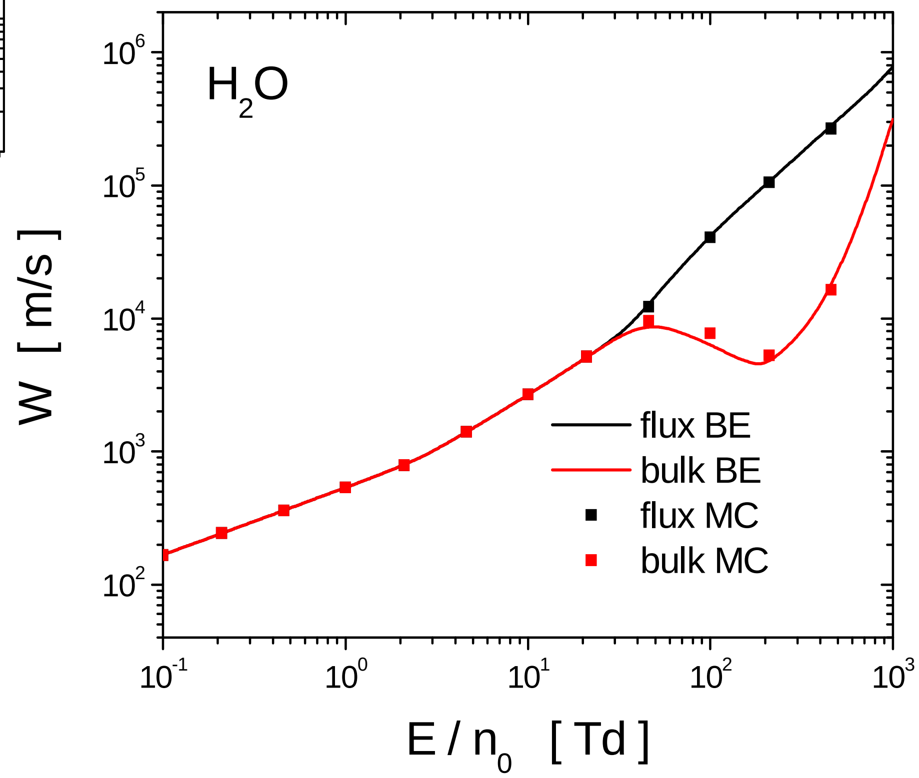


N_2 is a better choice for buffer gas in collisional traps than H_2!

Example – water vapour



The shape of the mean energy reflects the energy dependence of the cross sections

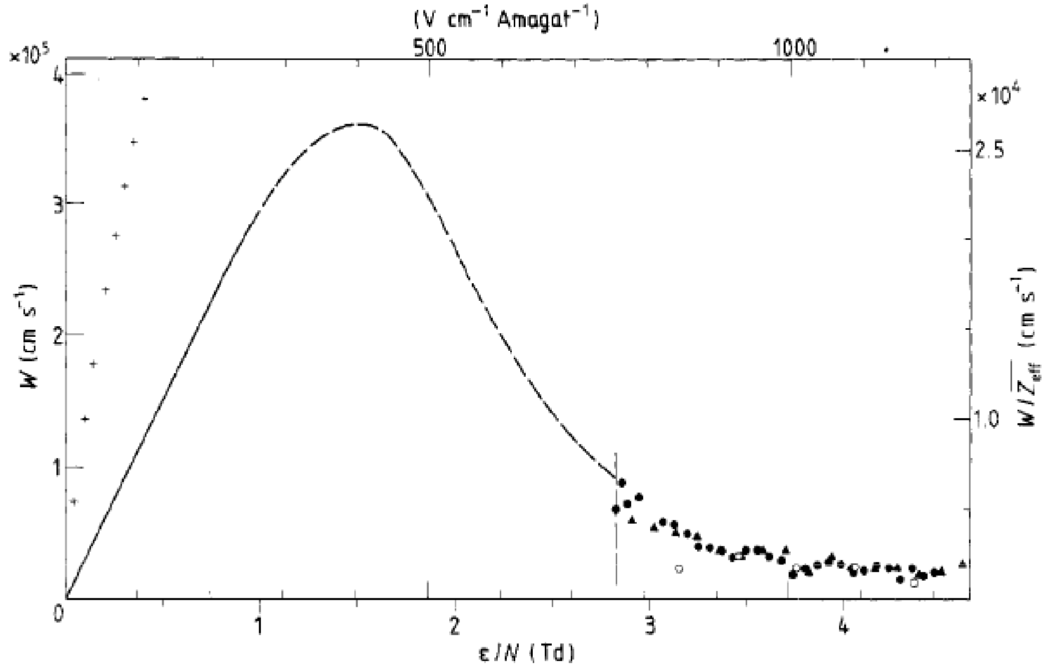


Huge difference between the flux and bulk components of the drift velocity!
Strong pronounced NDC!

Was any of this observed

Bose et al. J.Phys. B 14 (1981) L227

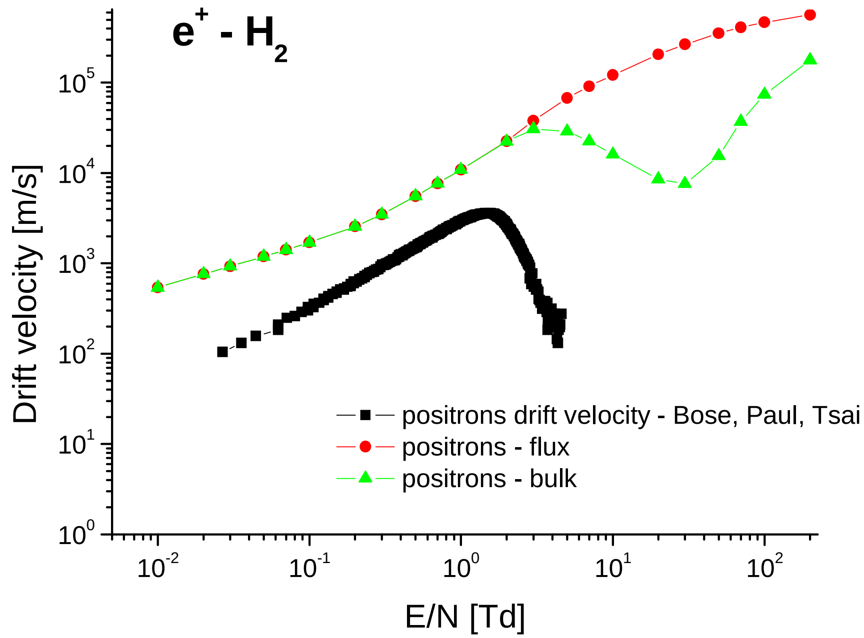
- Drift velocities (actualy w/Zeff) measured in H_2 show NDC, and flux drift velocities do not



- MC simulation of lifetime spectra contains mobility edge:

Farazdel Phys. Rev. Lett. 57(1986)2664

ble to that of the best available experiments. In the present work an additional energy threshold, namely the positron mobility edge E_c^+, is added to the FE simulation. Below E_c^+ the electric field is "turned off" until the positron reaches E_R below which it forms the cluster. The mobility edge is assumed to have no effect on the form of the collision cross sections involved. The input



e+ - H2
Drift velocity [m/s]
E/N [Td]
positrons drift velocity - Bose, Paul, Tsai
positrons - flux
positrons - bulk

What else is there?

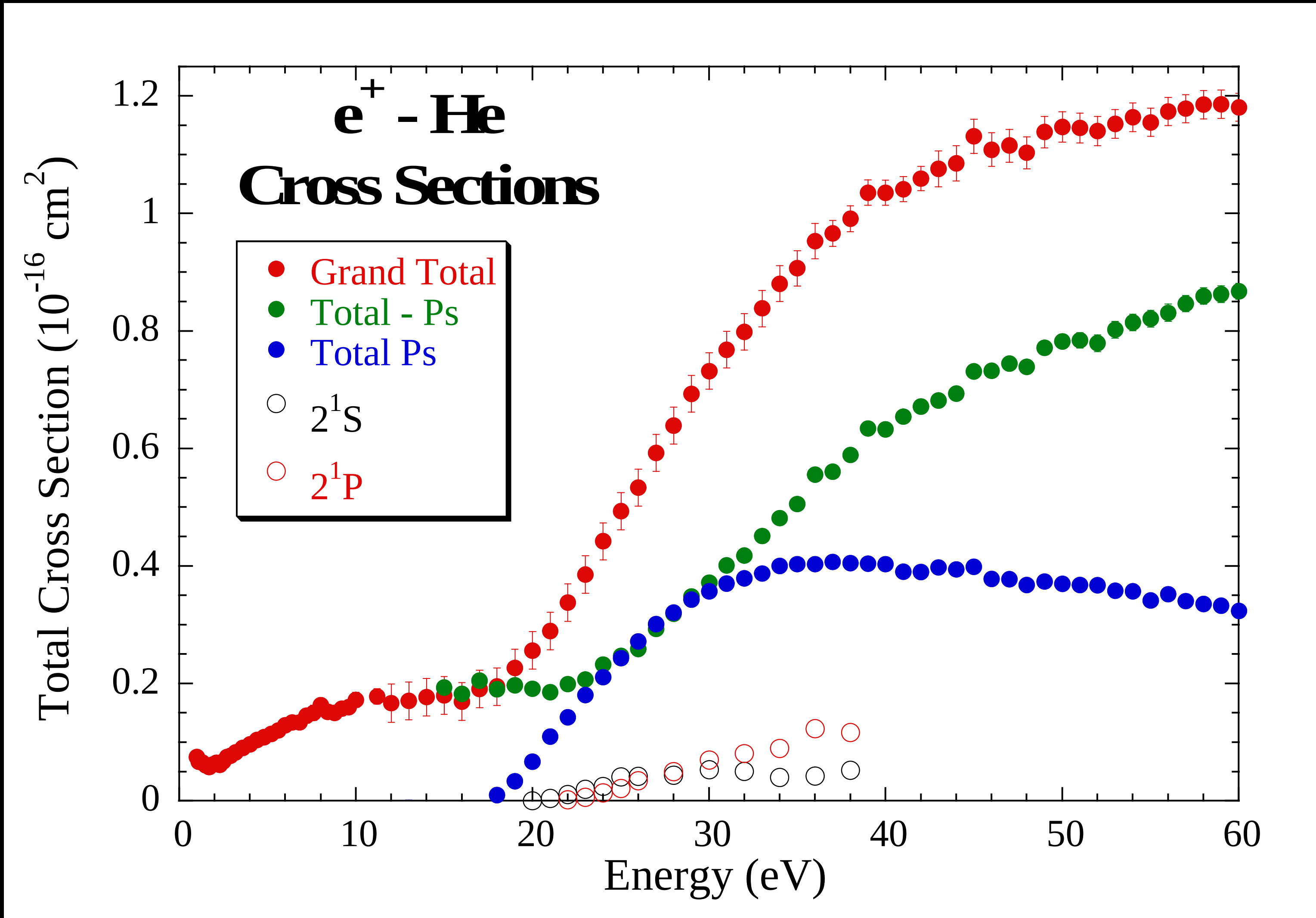
(Apart from the known and the unknown-Harold Pinter)

Molecular targets,

- Hydrogen Argon Nitrogen Water vapour
- $CF_4(+N_2)$

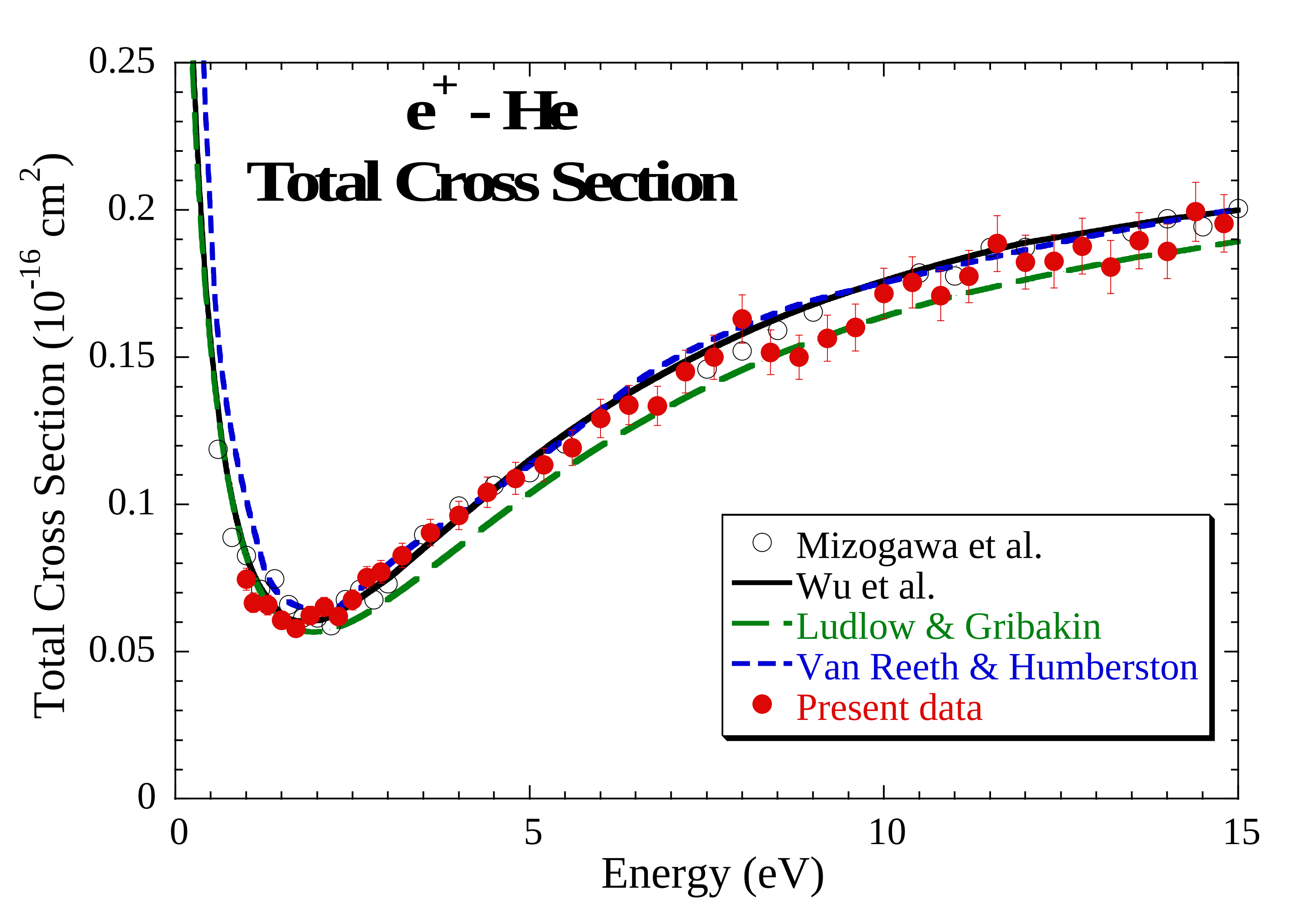
- Possibly O_2 CO hydrocarbons SF_6
- … protein like, DNA like

Atomic Cross Sections



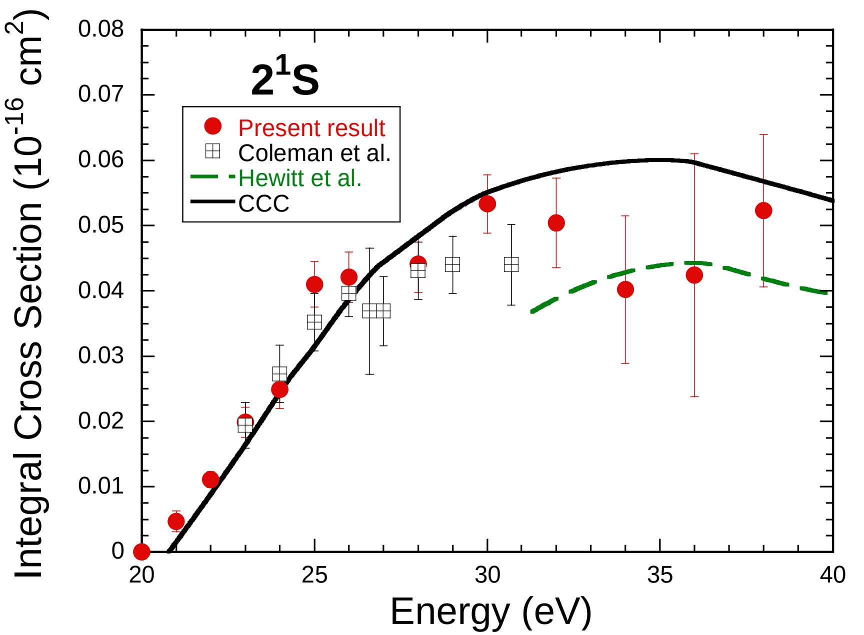
Phys. Rev. A **80** 032710 (2009)

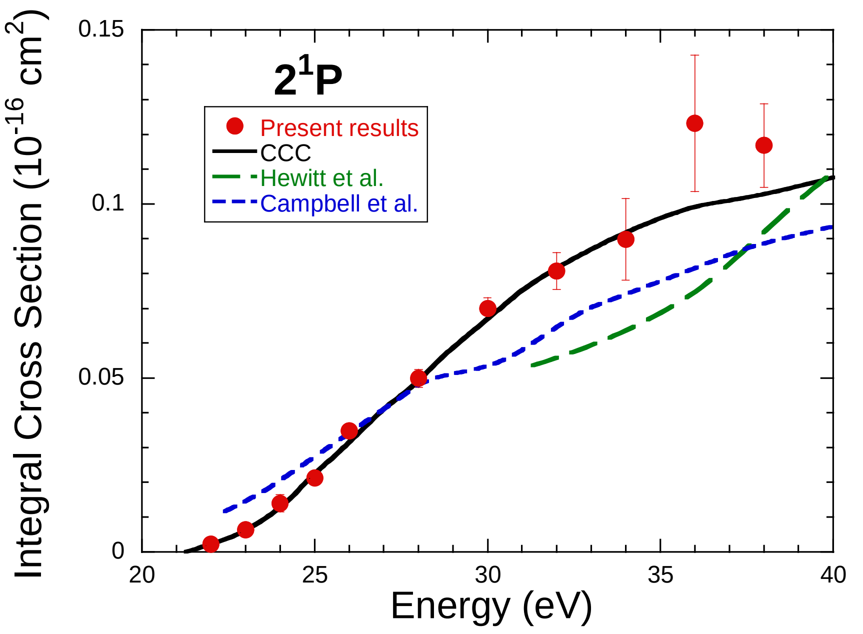
He – total scattering

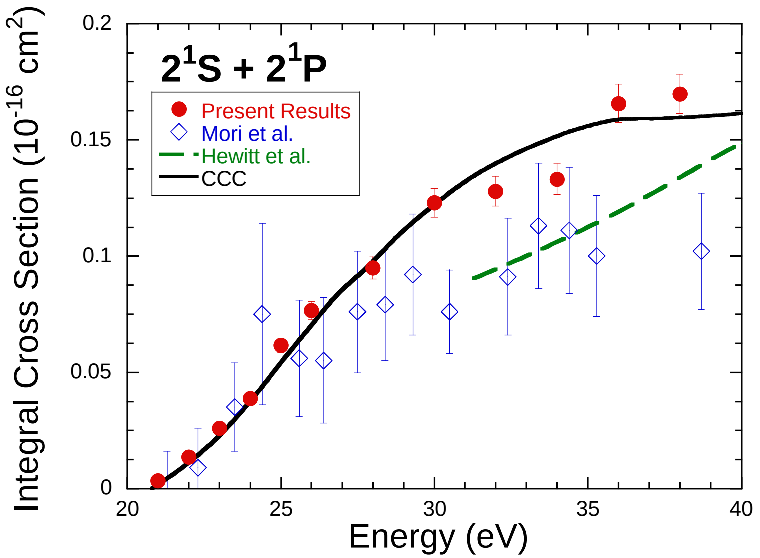


Phys. Rev. A **80** 032710 (2009)

He – electronic excitation



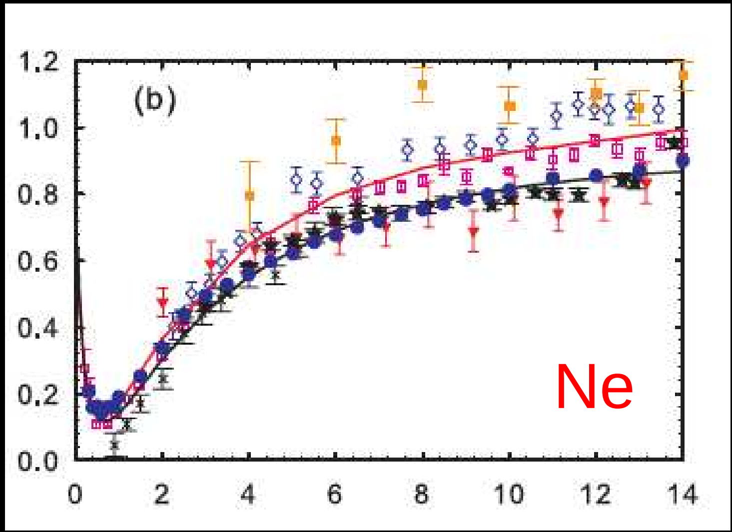


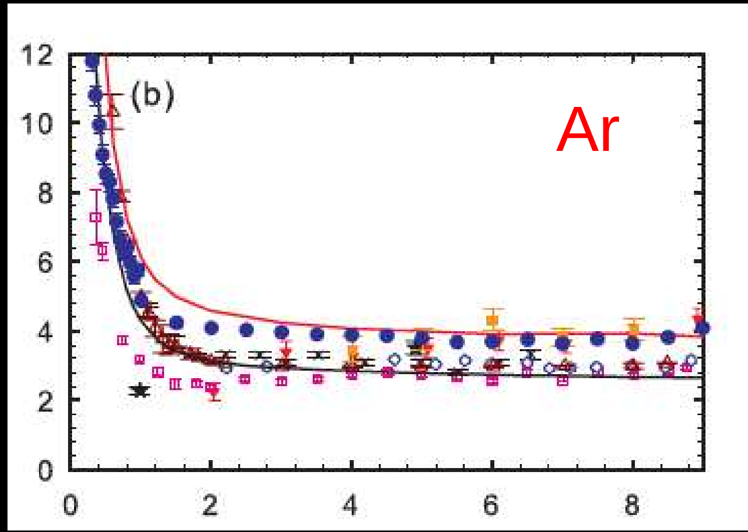


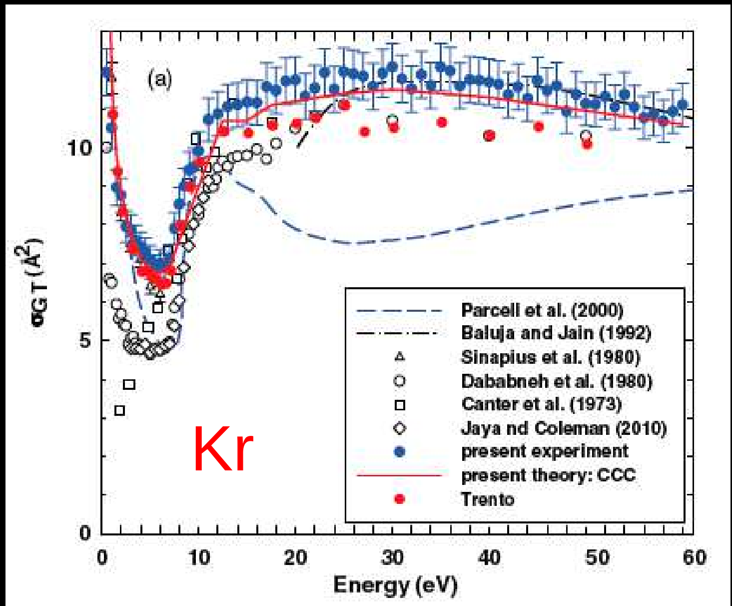
Caradonna et al.
PRA, 2009

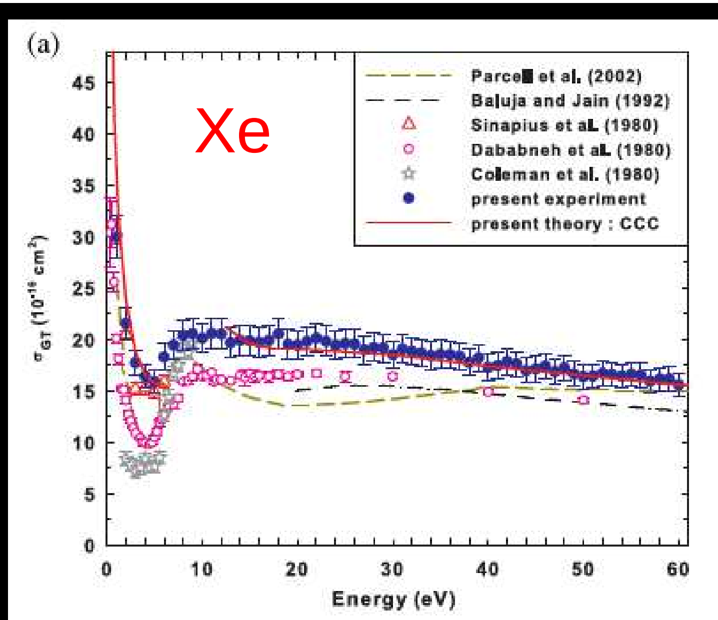
Theory
Utamuratov et al.
2009

Total Scattering Ne, Ar, Kr, Xe





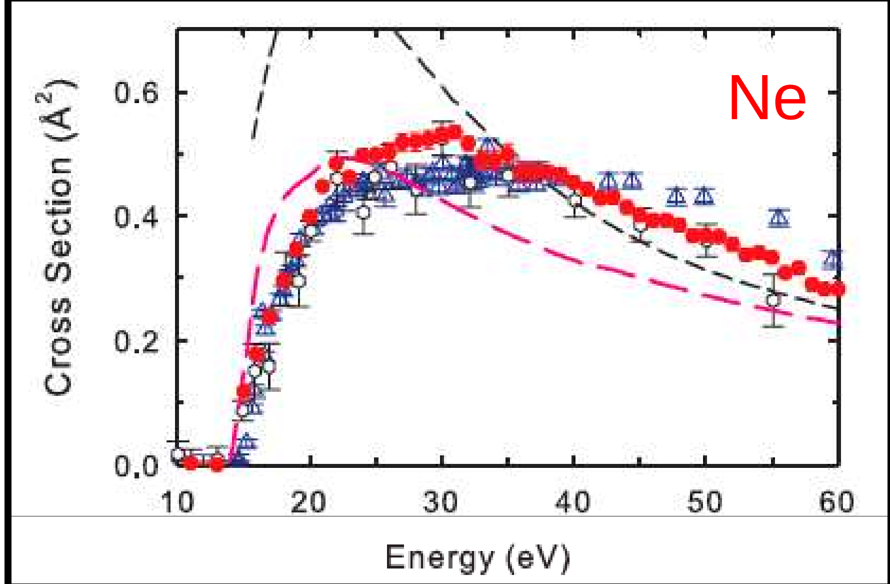


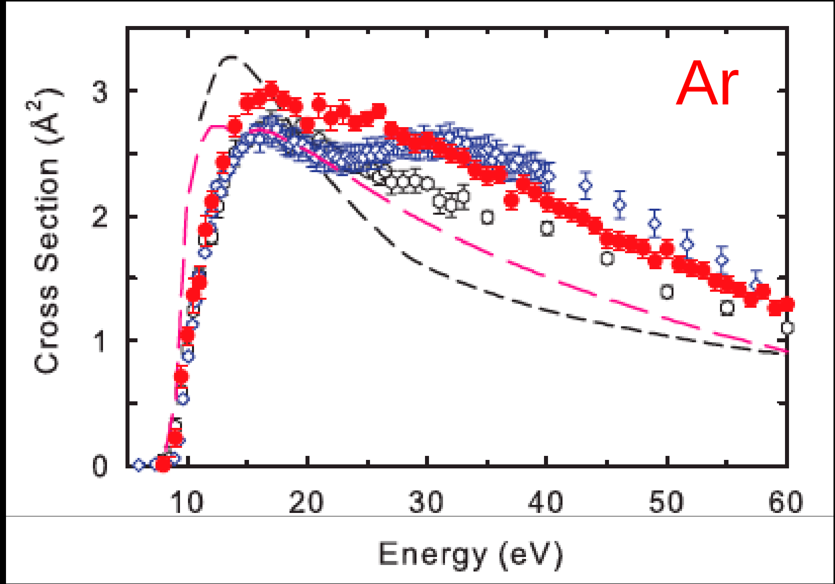


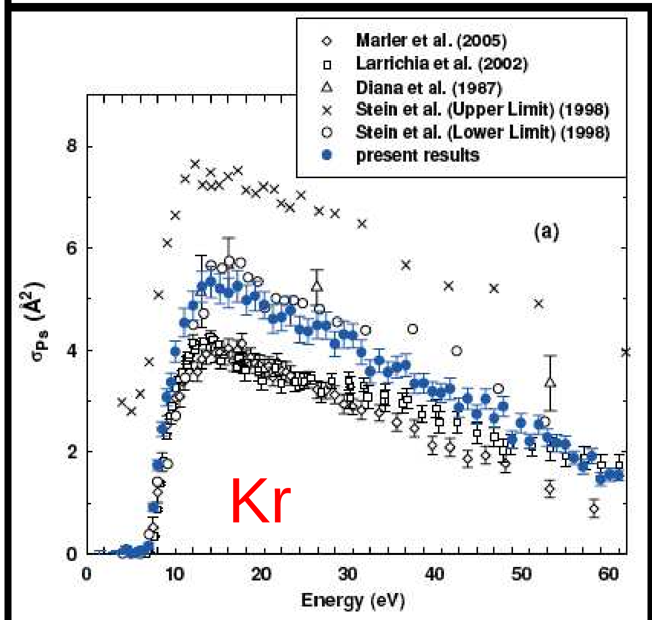
Phys. Rev. A**83** 032701 (2011)

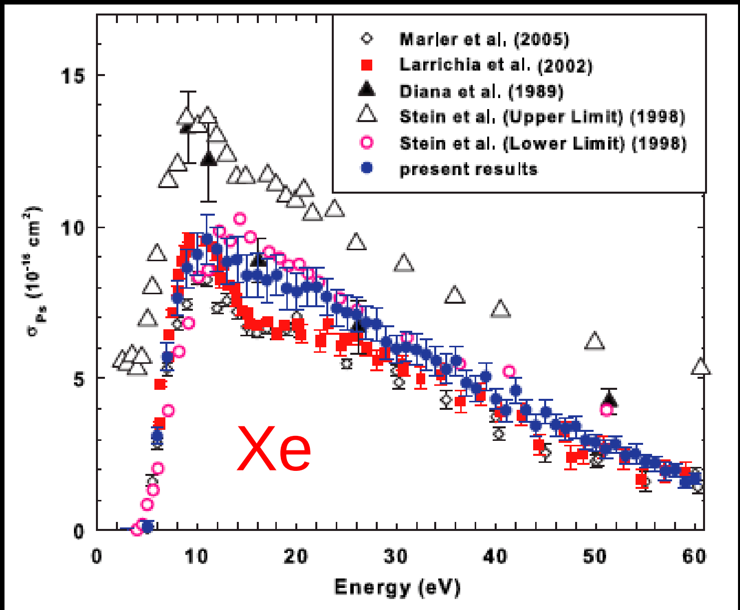
Phys. Rev. A**83** 032721 (2011)

Ps Formation Ne, Ar, Kr, Xe





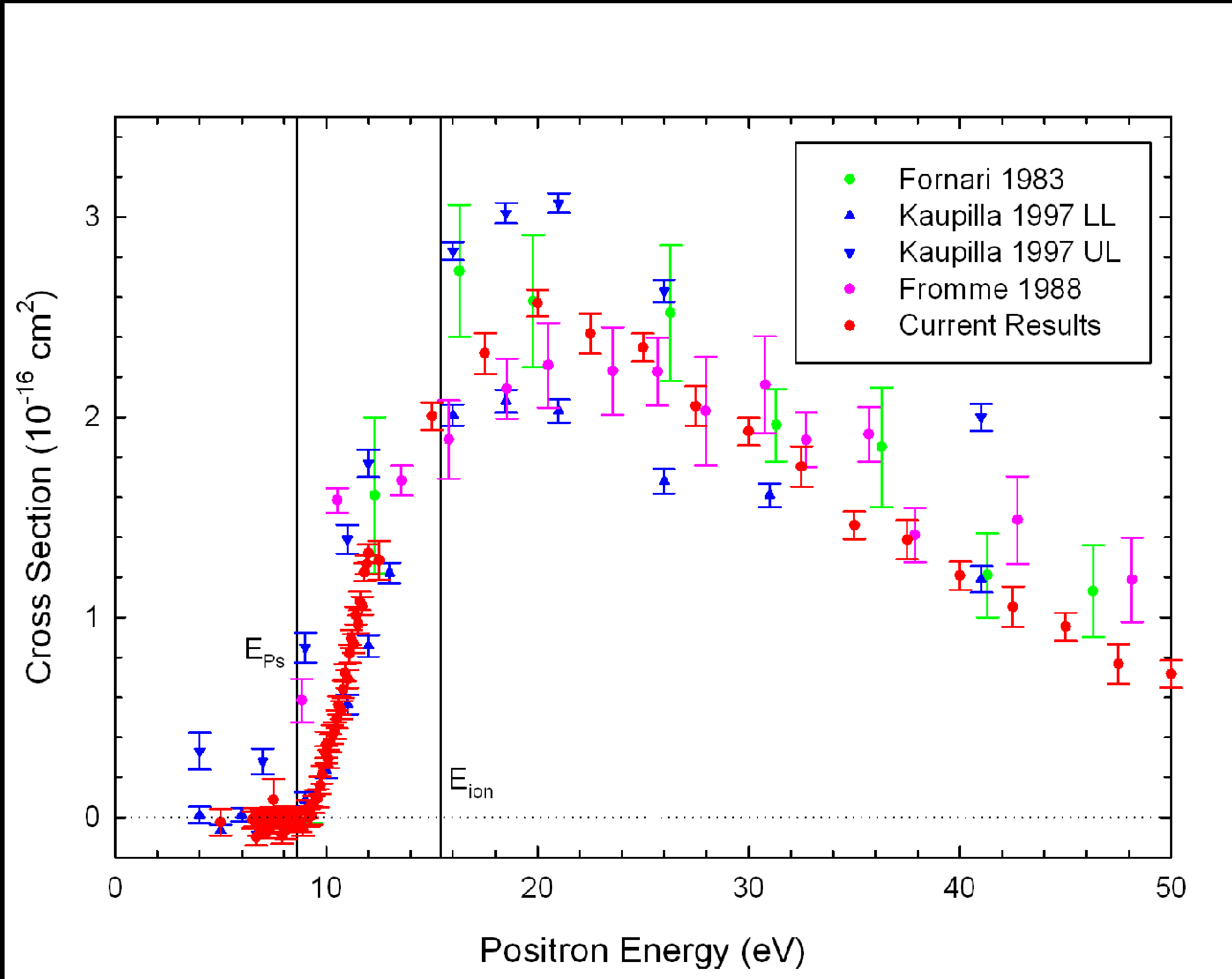




Phys. Rev. A**83** 032701 (2011)

Phys. Rev. A**83** 032721 (2011)

$Ps - H_2$



Fornari 1983
Kaupilla 1997 LL
Kaupilla 1997 UL
Fromme 1988
Current Results
Cross Section (10^-16 cm^2)
Positron Energy (eV)
E_Ps
E_ion
0
1
2
3
0
10
20
30
40
50

Available data:

- Ps formation
- direct and total ionization
- $A^1\Pi$ electronic excitation
- vibration v1
- total cross section (theoretical 10-5000 eV)
- differential for elastic (+ vib + rot)

CO

Missing data:
other electronic and vibrational excitations

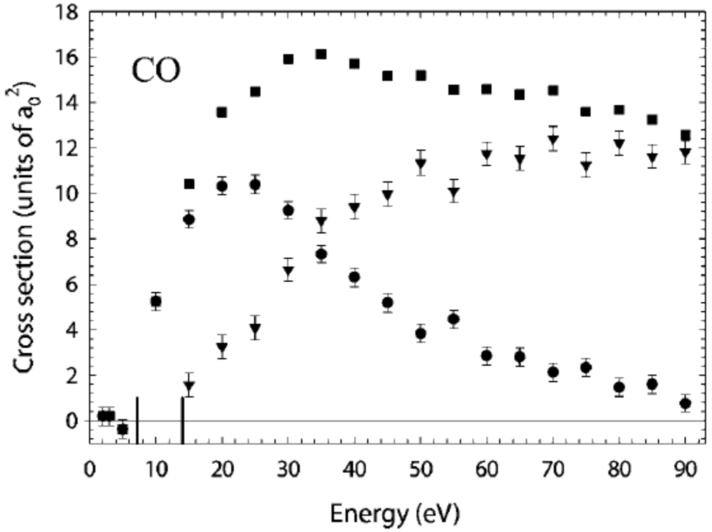


FIG. 6. Integral cross sections for CO: (●) positronium formation, (▼) direct ionization, and (■) total ionization.

Marler & Surko, PRA 72 (2005) 062713

Marler & Surko, PRA 72 (2005) 062713

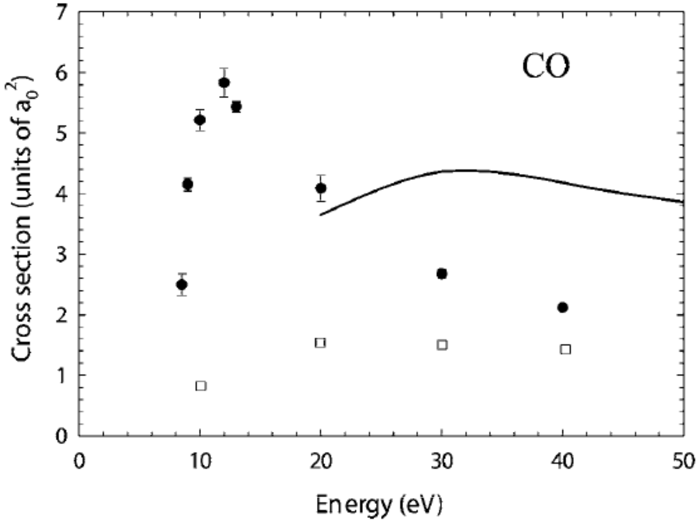
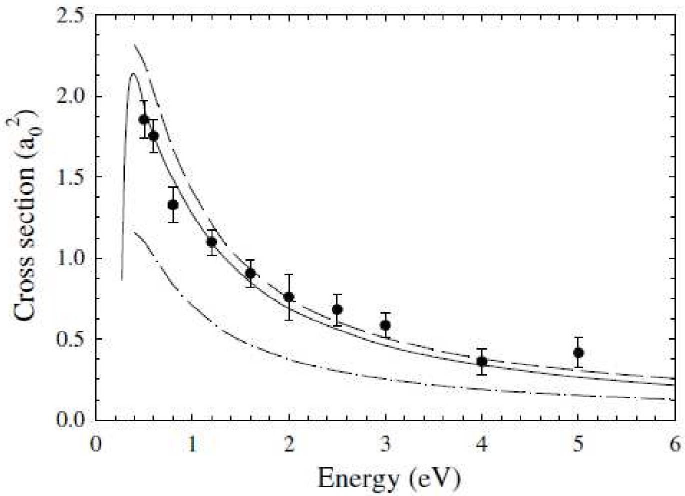


FIG. 13. Integral cross sections for the excitation of the $A\ ^1\Pi$ state in CO by (●) positron and (□) electron impact [28]. Also



v1 vibrational mode of CO. Sullivan, Gilbert & Surko, PRL 86 (2001) 1494

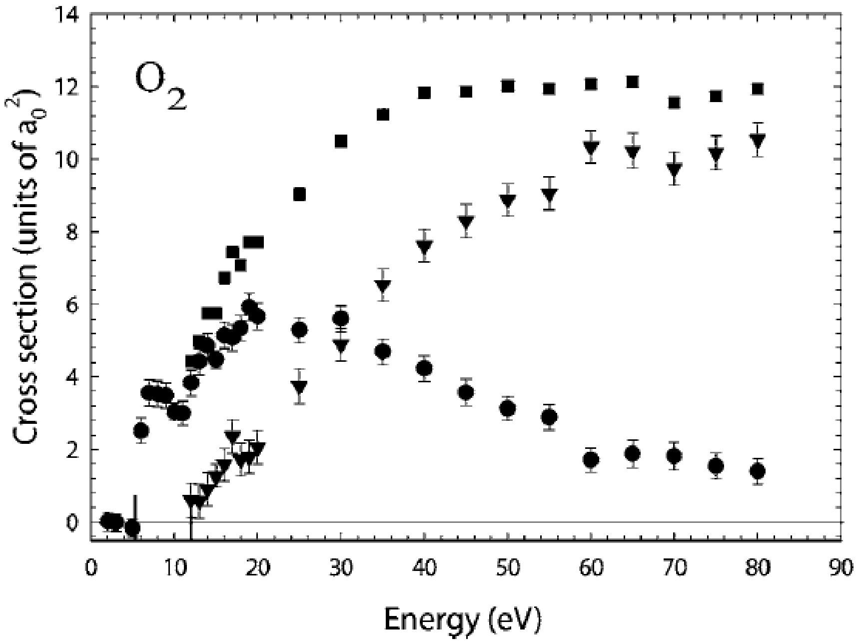
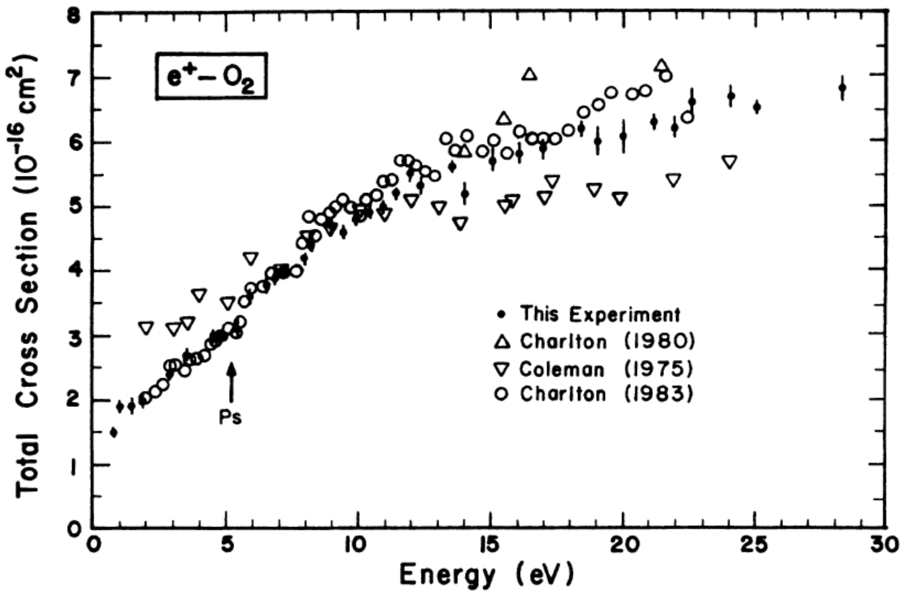


FIG. 8. Integral cross sections for O_2: (●) positronium formation, (▼) direct ionization, and (■) total ionization.

Marler & Surko, PRA 72 (2005) 062713



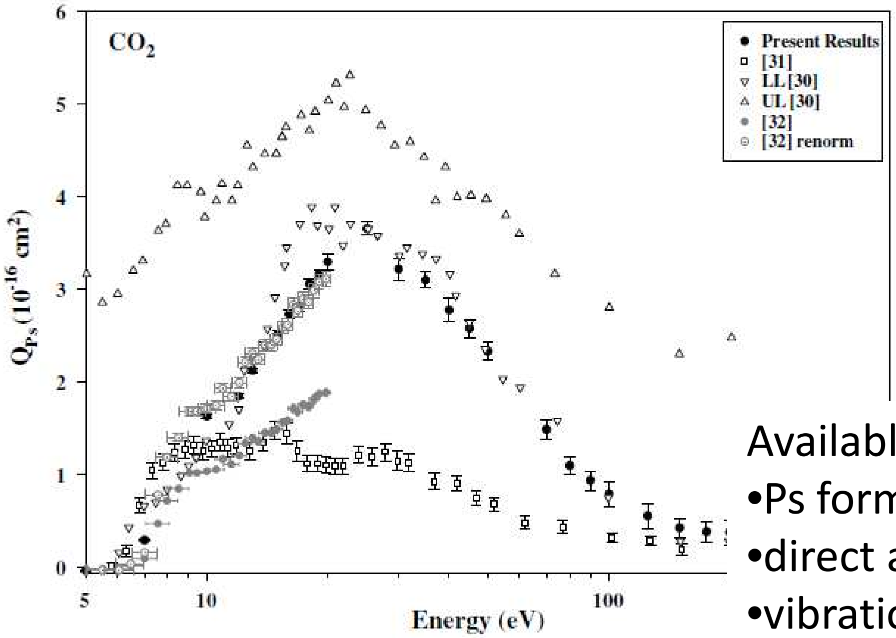
Dababneh et al., PRA 38 (1988) 1207

O_2

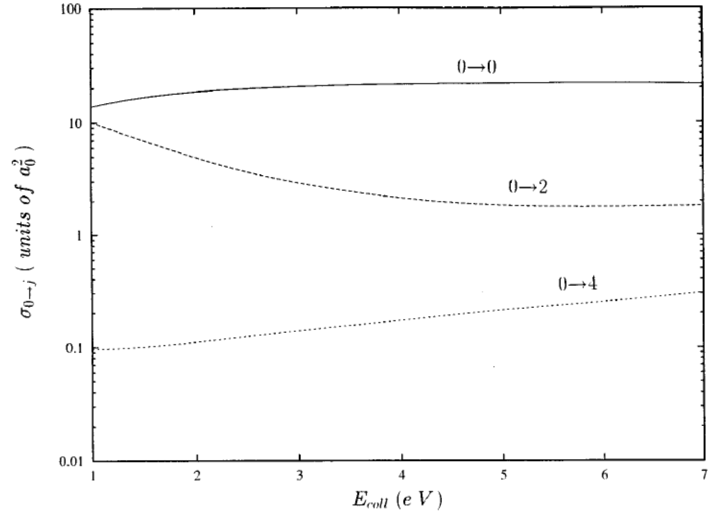
Available data:
- Ps formation
- direct and total ionization
- vibration v1
- total cross section (experimental measurements at low energies and theoretical calculations in the range 10-5000 eV)
- differential for elastic (+ vib + rot)

Missing data:
- electronic excitations
- vibrational excitations
- rotational excitations

CO_2

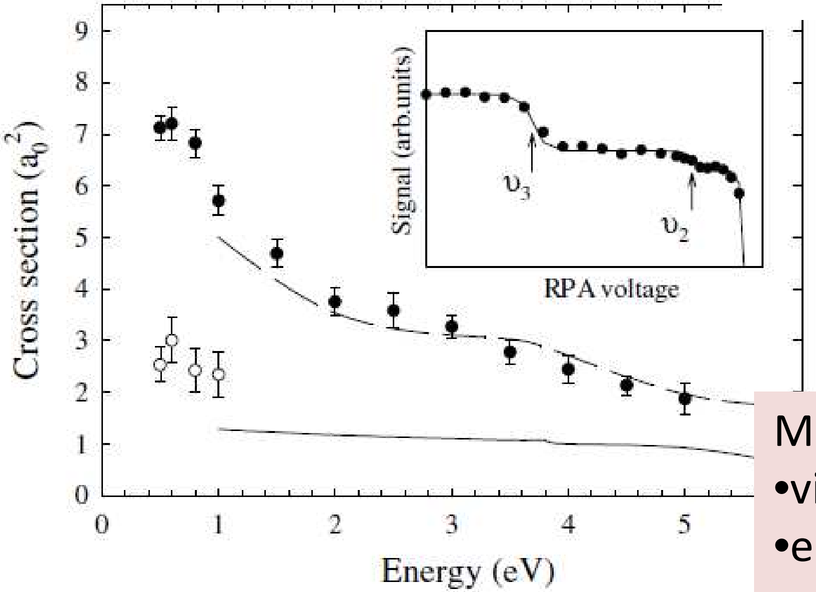


Murtagh *et al*, NIMB 247 (2006) 92



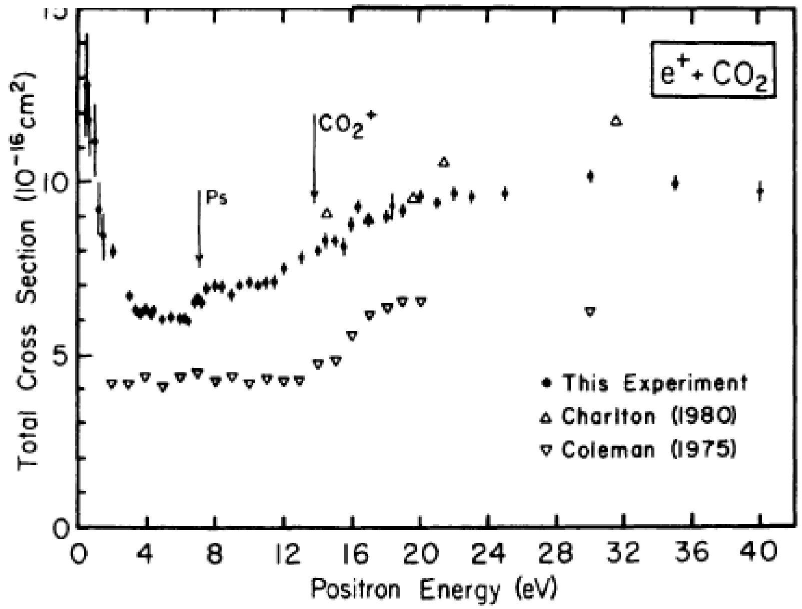
Rotational cs
Gianturco & Paioletti, PRA 55 (1997) 3491

Available data:
- Ps formation
- direct and total ionization
- vibration v2 and v3
- total cross section
- differential for elastic (+ vib + rot)



v2 and V3 vibrational mode of CO_2.
Sullivan, Gilbert & Surko, PRL 86 (2001) 1494

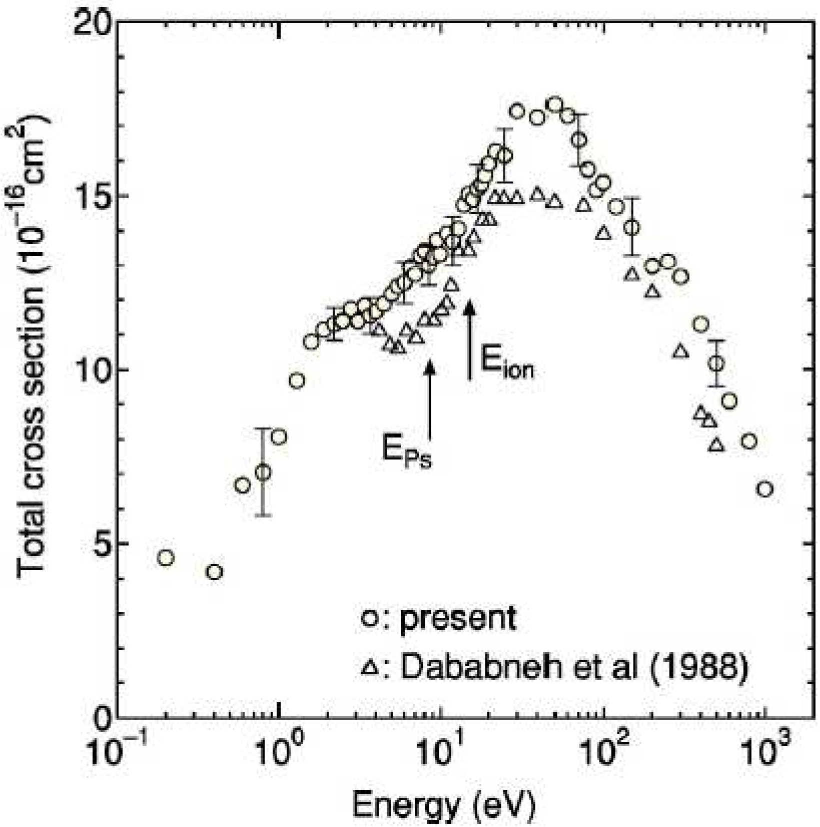
Missing data:
- vibration v1
- electronic excitations



Hoffman et al., PRA 25 (1982) 1393

SF_6

Important in applications of rotating wall technique.



Total cs.
Makochekanwa, Kimura & Sueoka, PRA 70 (2004) 022702

The only available data in literature is on total cross section!

Missing data:
- Ps formation
- direct and total ionization
- electronic excitations
- vibrational excitations
- differential cross sections

CHOOH (formic acid)

CAMS measurements:

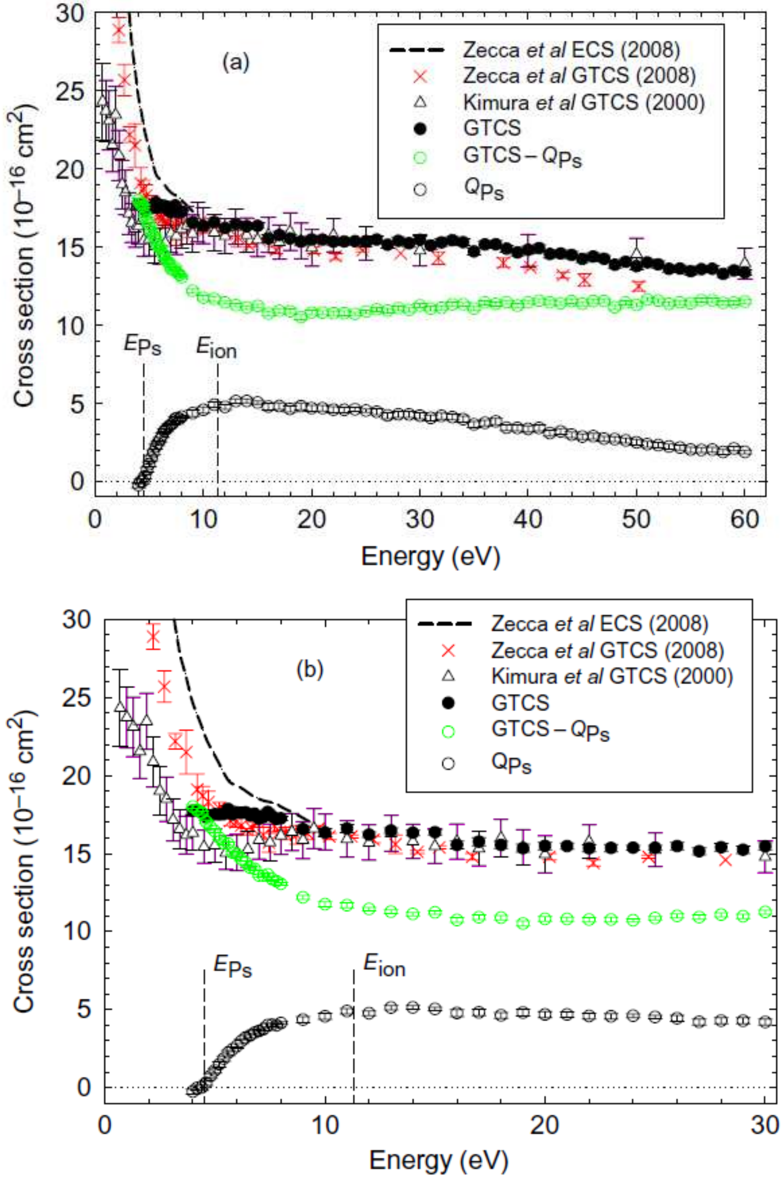


Figure 6. Present positron impact HCOOH GTCS, GTCS − Q_{Ps} and Q_{Ps} compared with literature for GTCS and elastic integral (ECS) results (a) over the whole energy range of measurement and (b) below 30 eV.

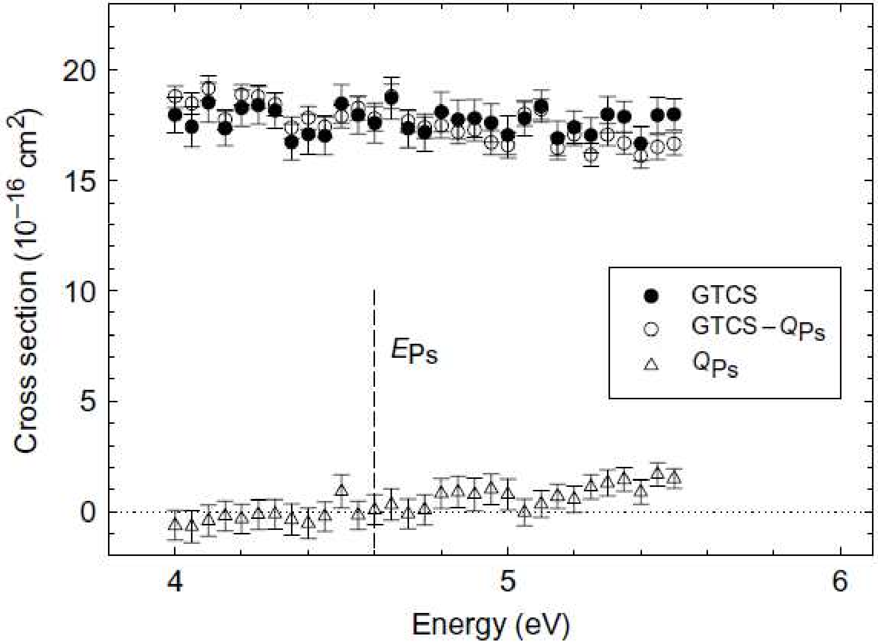
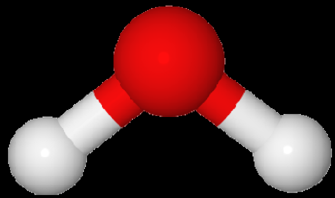


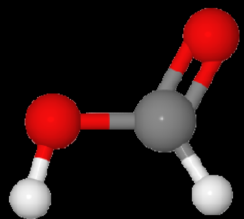
Figure 7. Present positron impact HCOOH GTCS, GTCS − Q_{Ps} and Q_{Ps} results in the vicinity of the Ps threshold ($E_{Ps} = 4.53$ eV).

Makochekanwa *et al.*, New J. Phys. 11 (2009) 103036

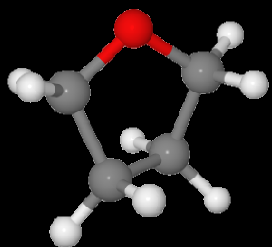
Ps – “Bio Molecules”



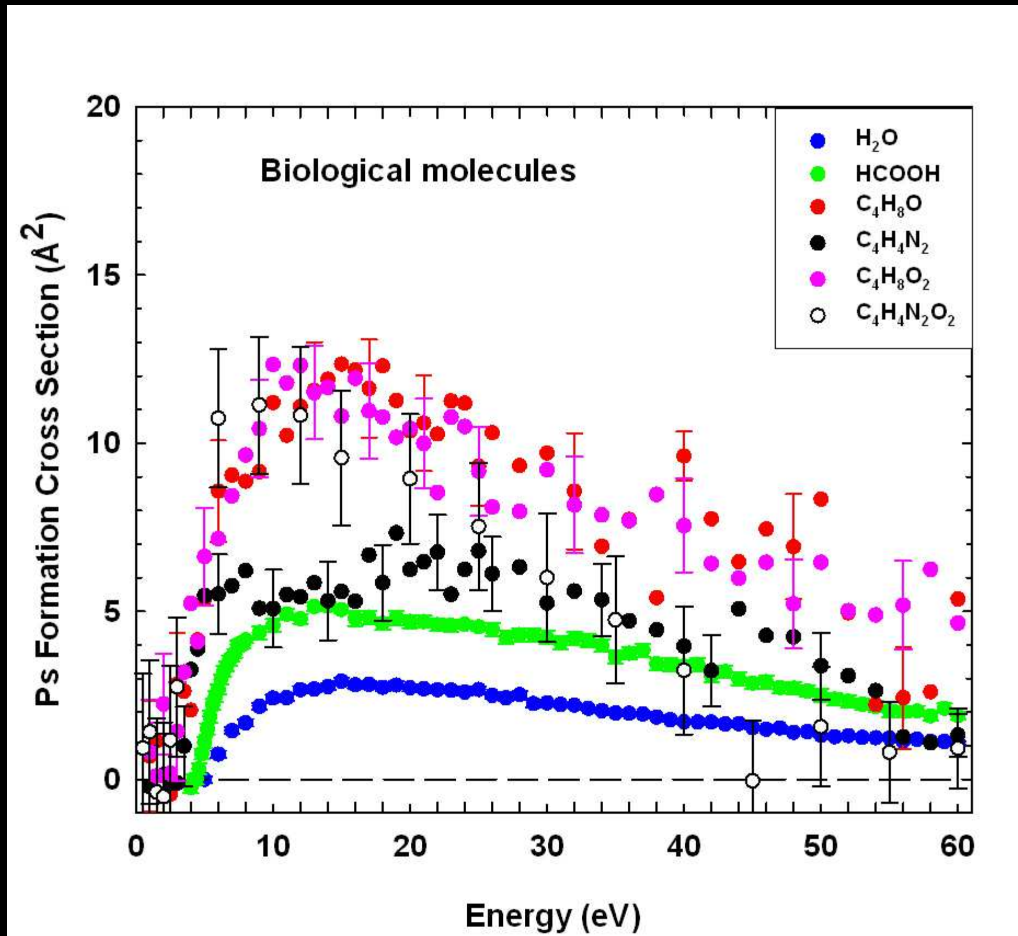
Water
10 electrons

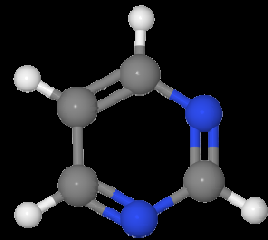


Formic Acid
25 electrons

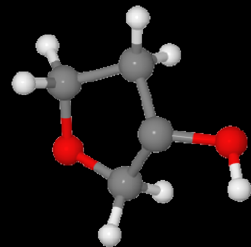


THF
40 electrons

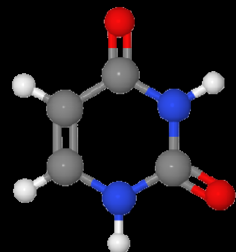




Pyrimidine
42 electrons

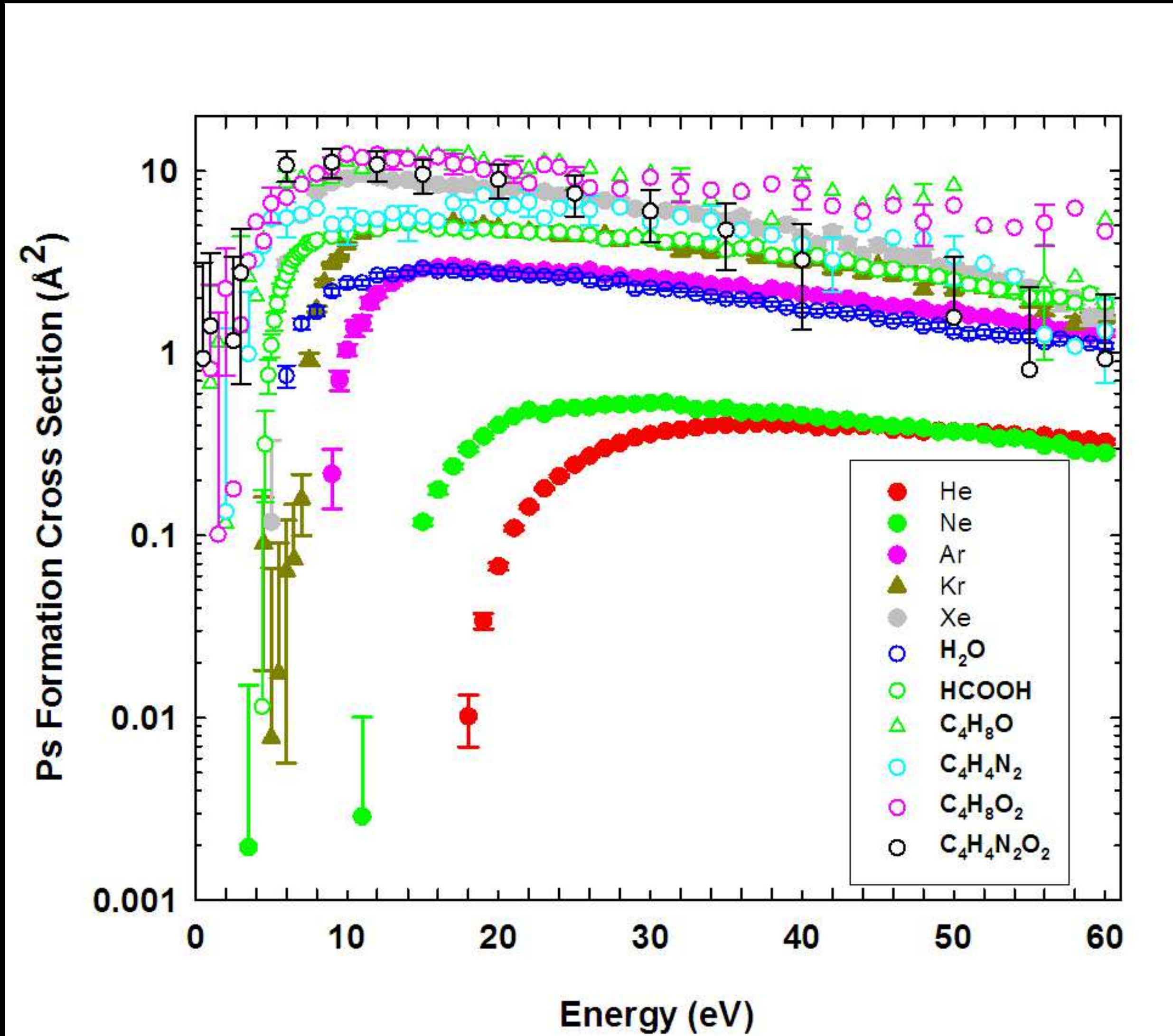


3h-THF
47 electrons

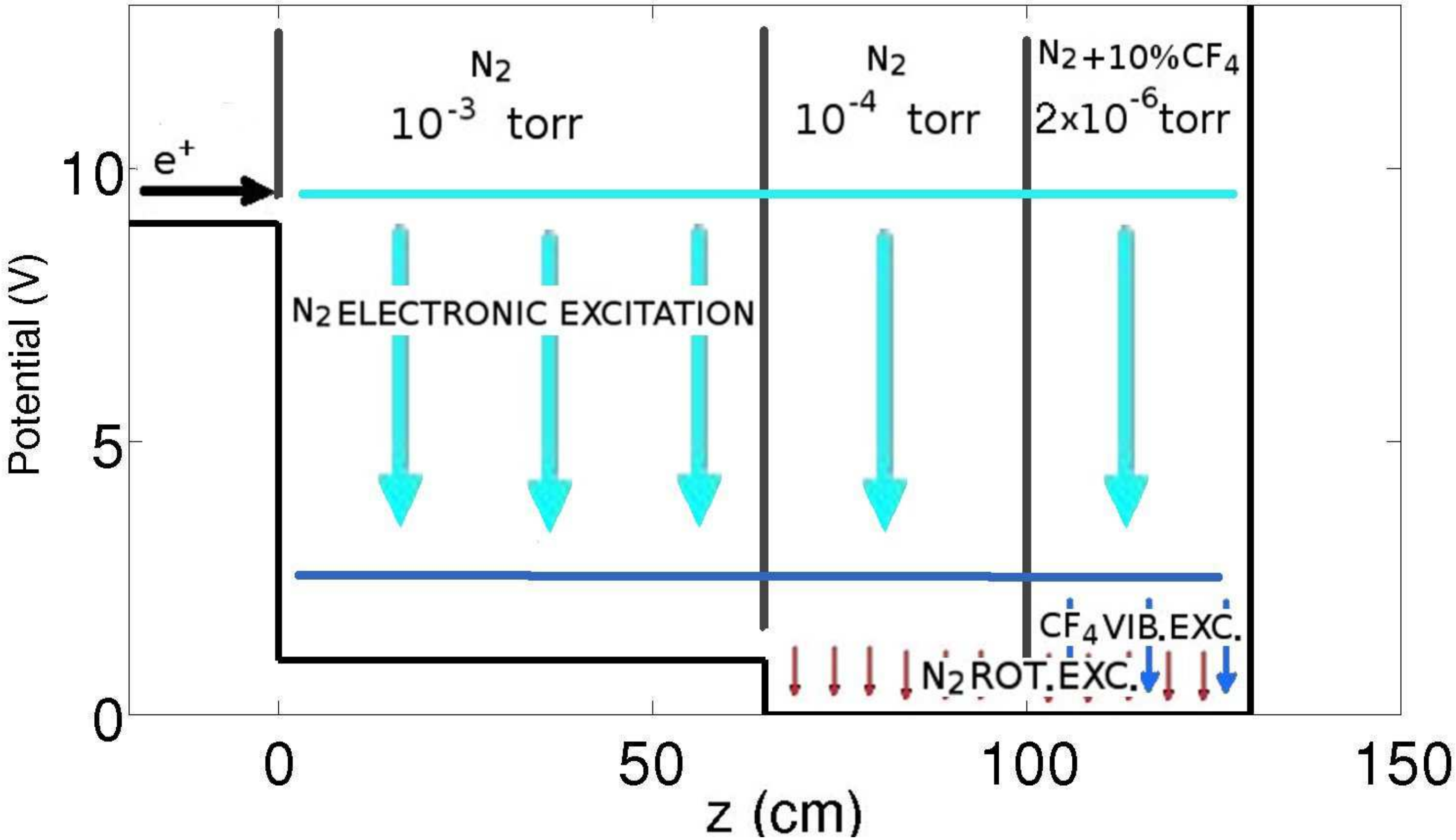


Uracil
58 electrons

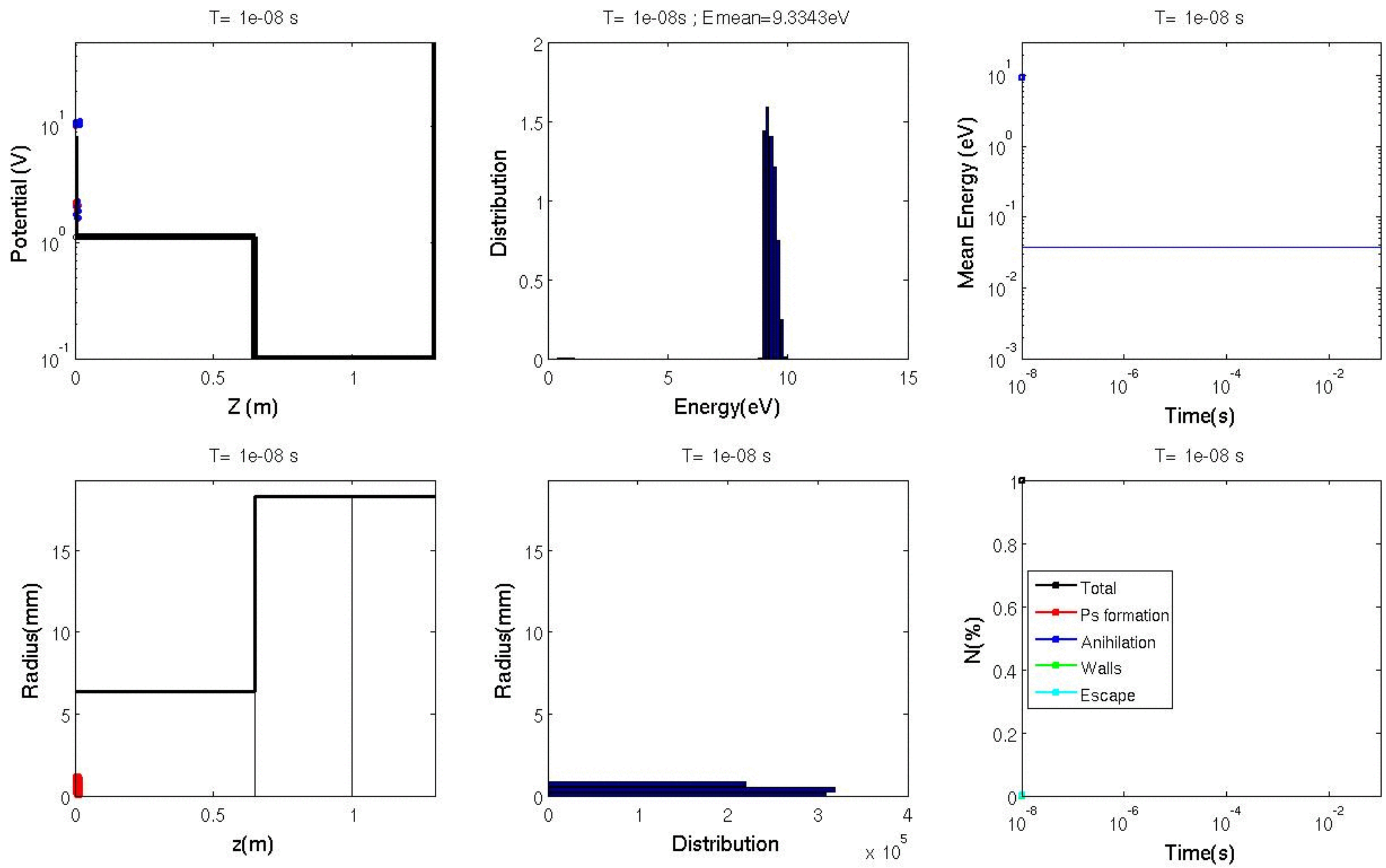
Ps- importance of structure



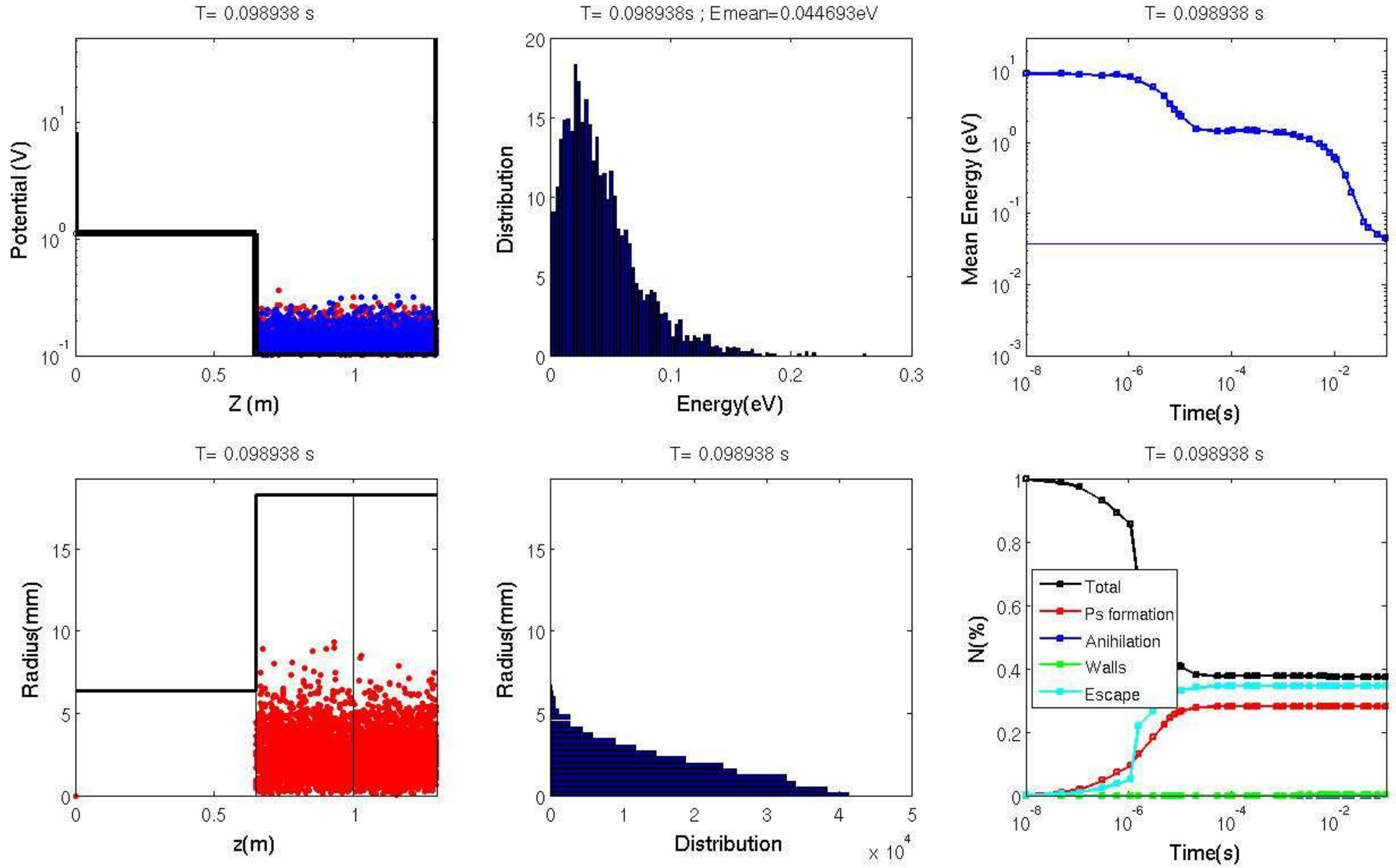
Application of data to model a Surko trap



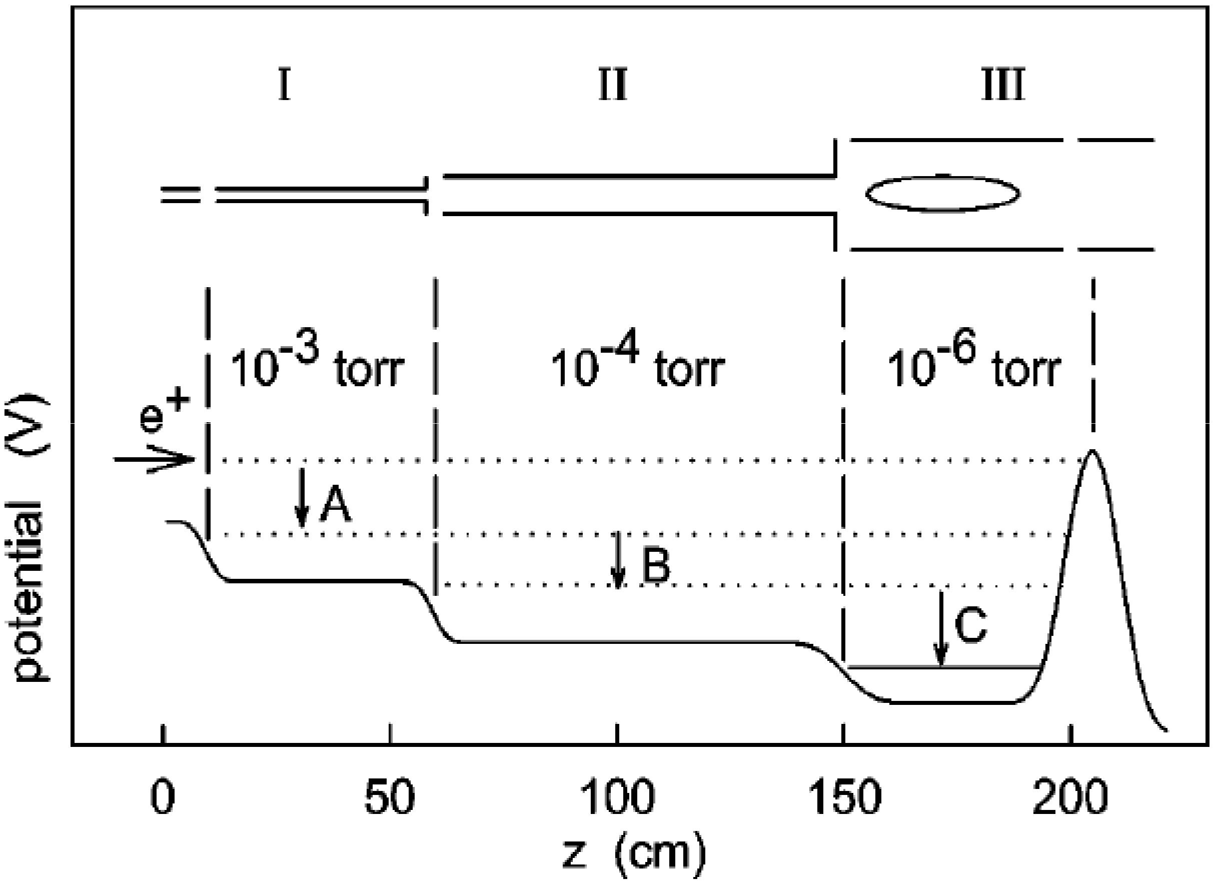
Standard Surko trap



Standard Surko trap



Rotating wall+
Penning Malmberg Surko trap



Harmonic potential

Plus

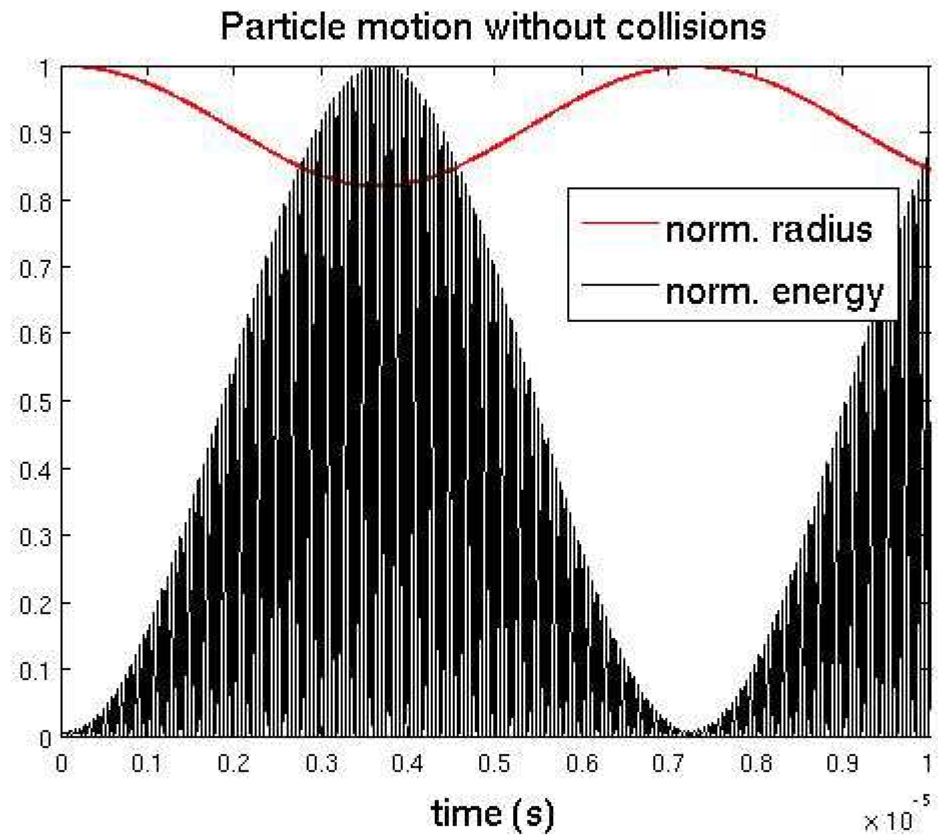
Strong gradient

Dipole or Quadrupole Rotating field

- N_2 , H_2 , CO , CO_2 , CF_4

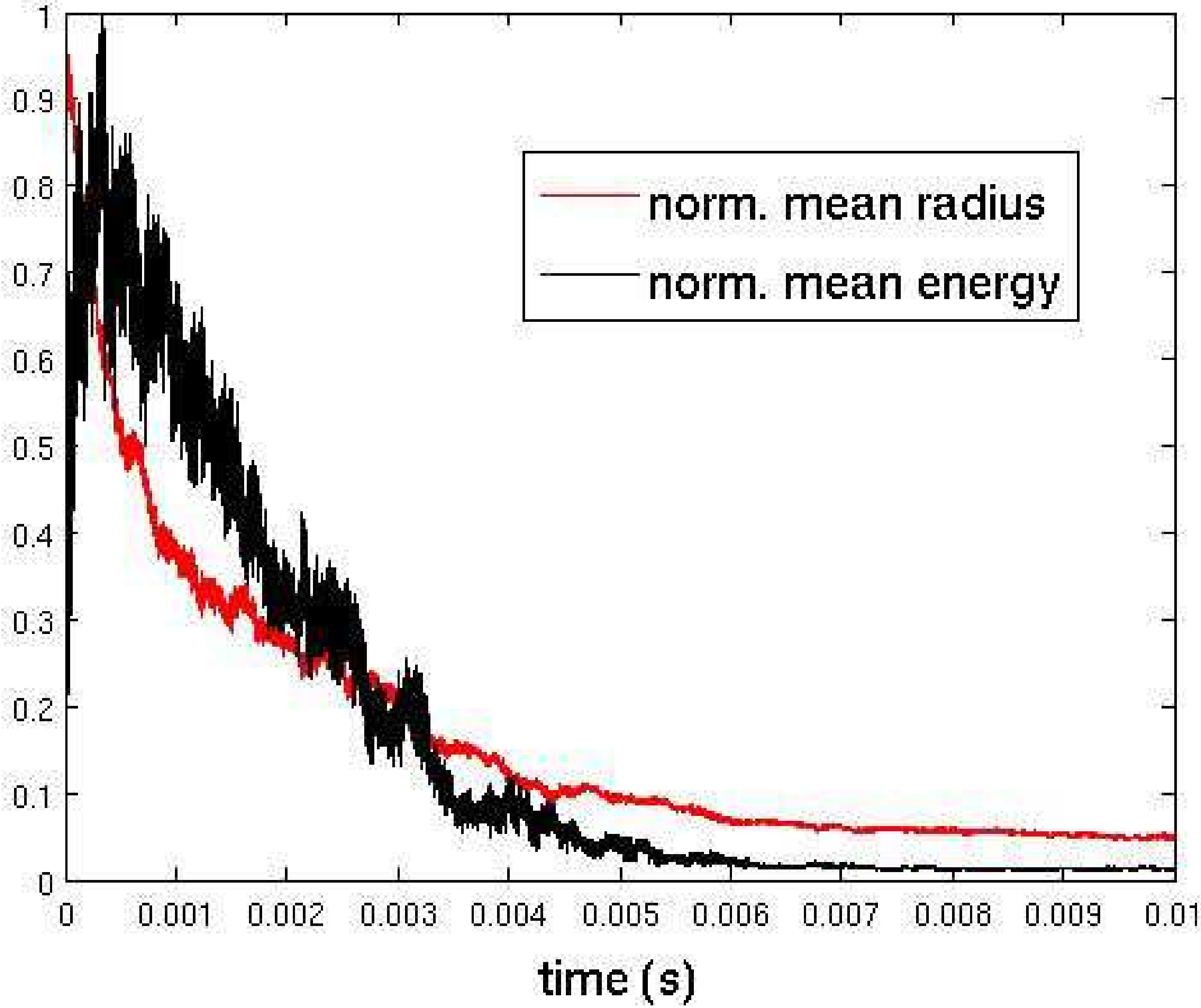
C. M. Surko and R. G. Greaves, **Phys. Plasmas 11**, 2333 (2004)

Rotating wall

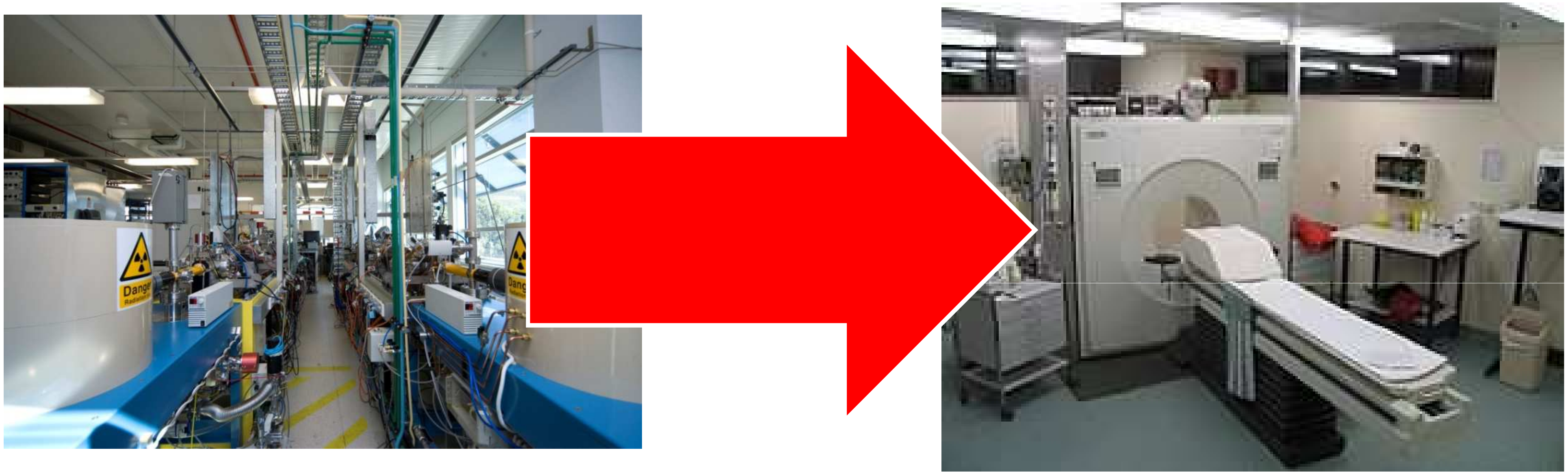


Collisions necessary
Gradient necessary

Rotating wall



Can we apply (sell) elementary AM-positron data for modelling of medical procedures (NIH)?



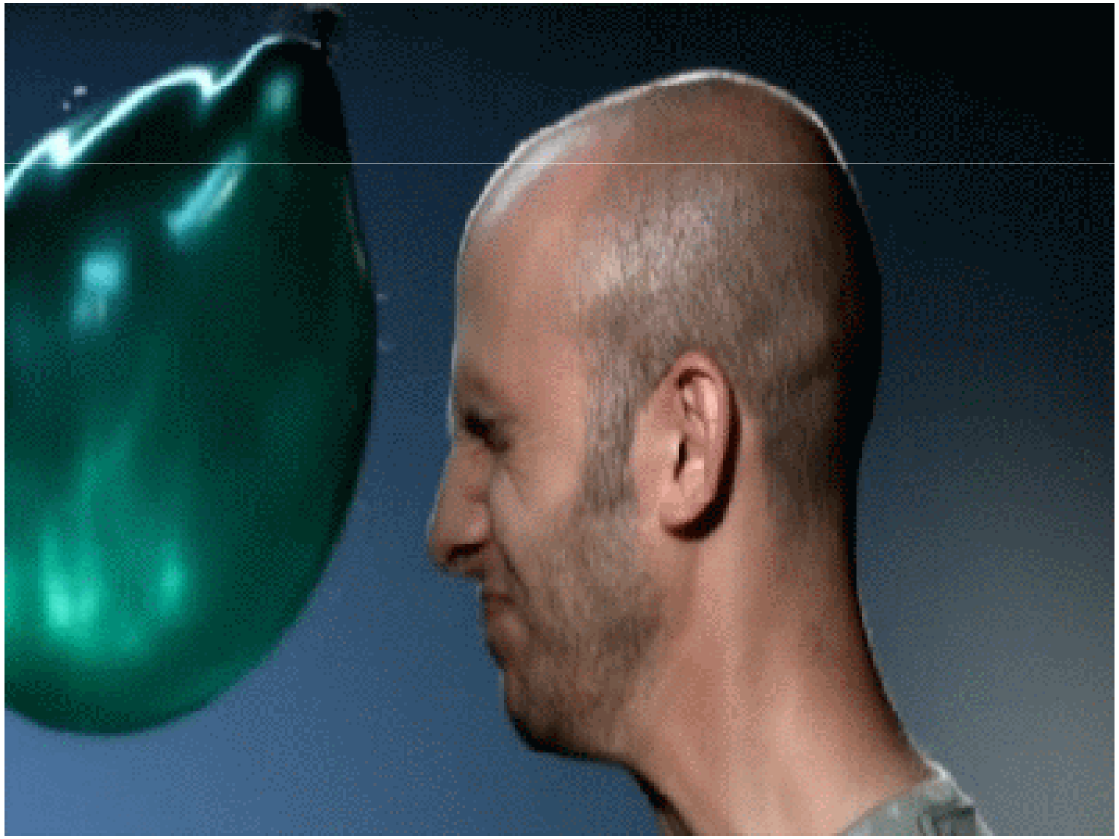
- we got water balloon model- water cross sections- tracks -transport coefficients etc.

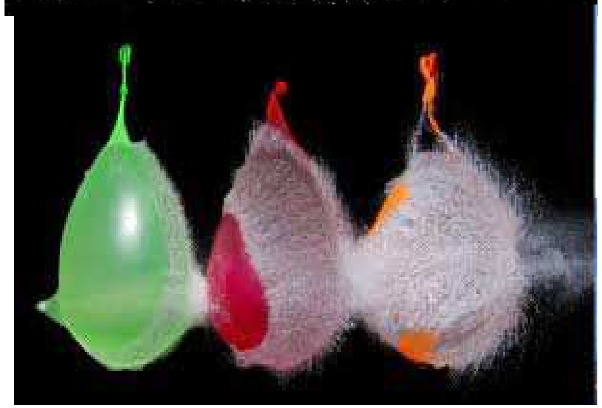
4th step: application of atomic data and models of ionized gases for PET and positron therapy

Medicine: science about human beings

and how to repair them

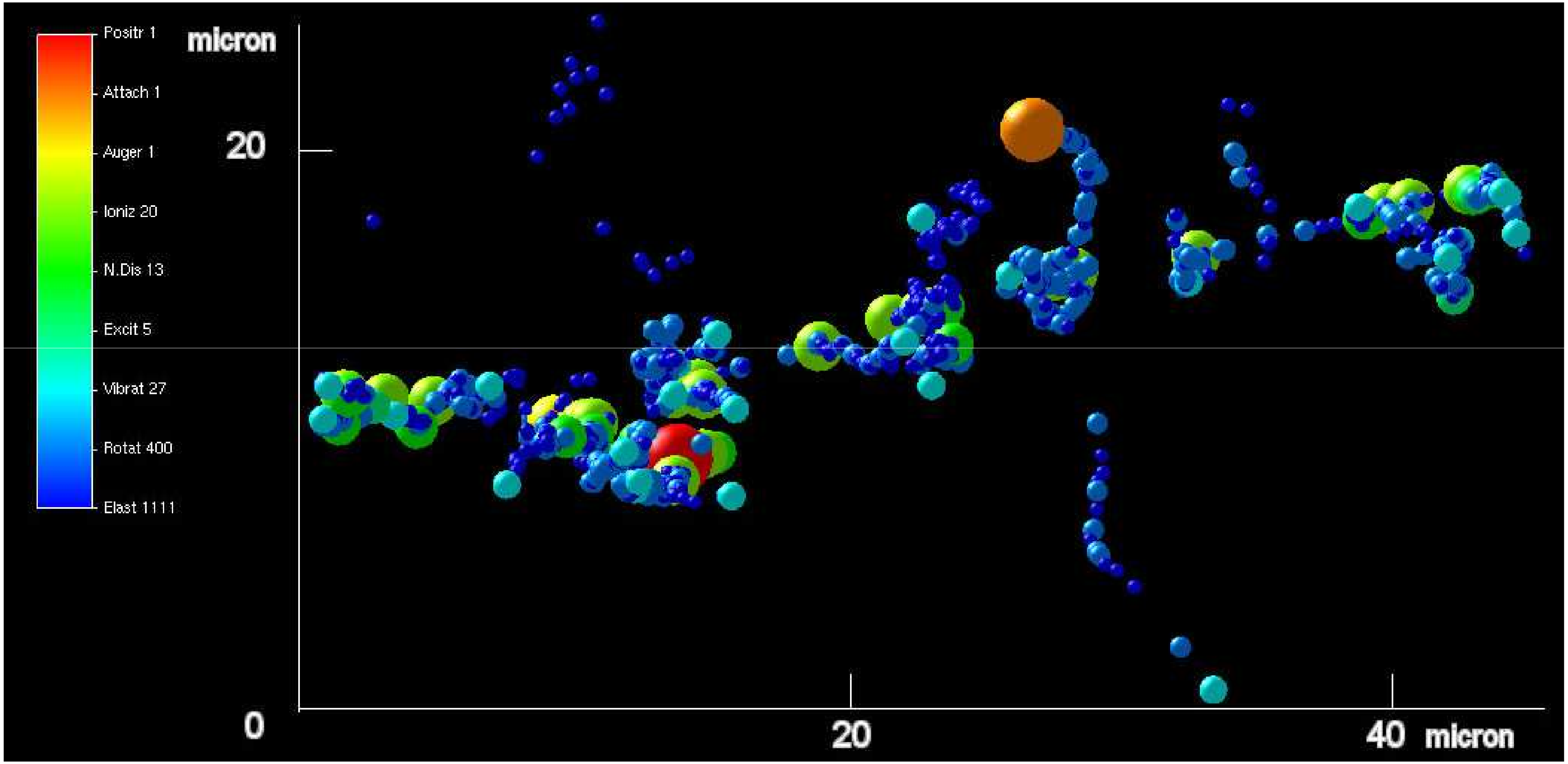
- What is a man/woman: a water (bag) balloon - in a tradition of a spherical cow



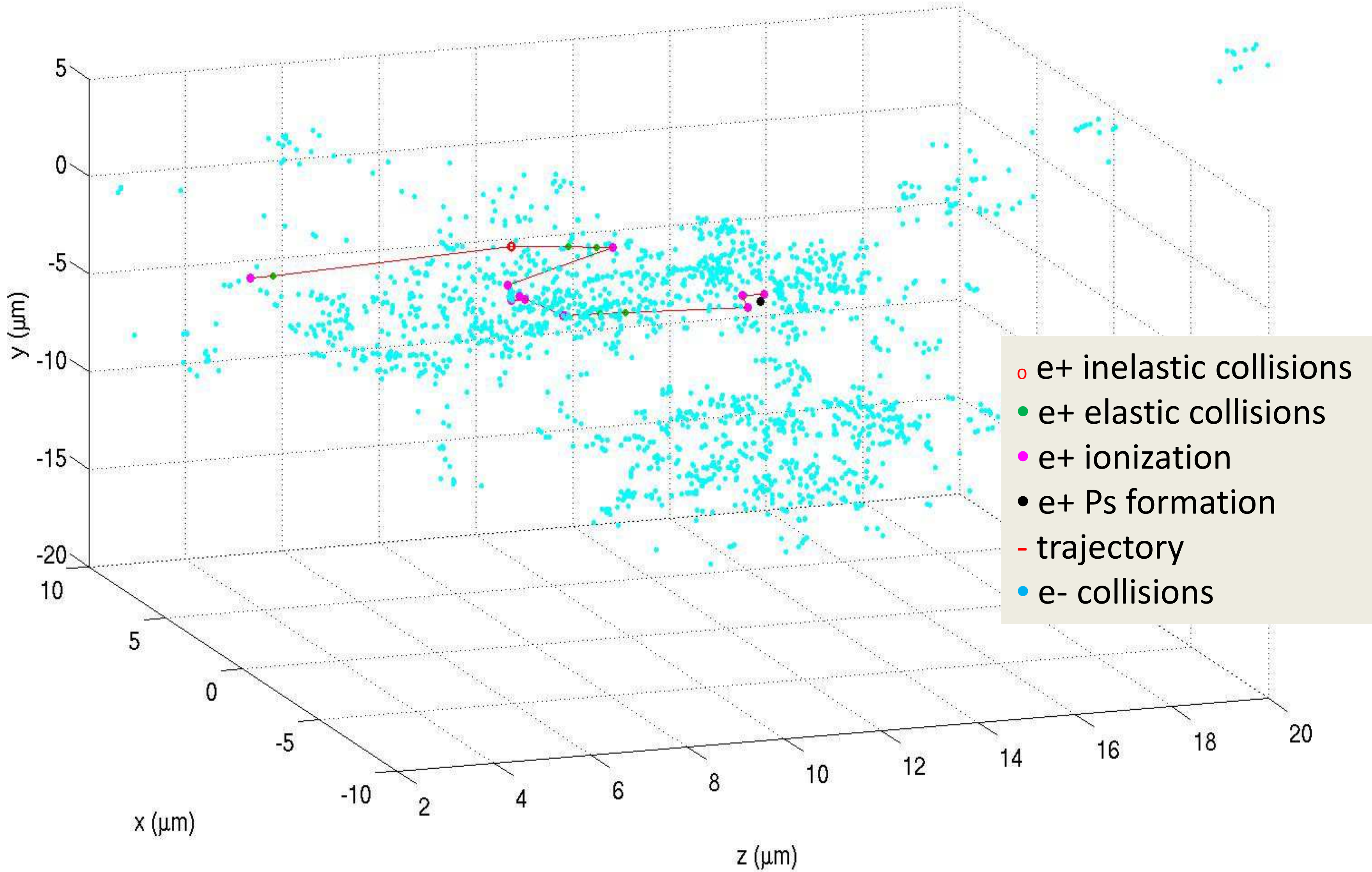


Dense gaseous medium
-transport

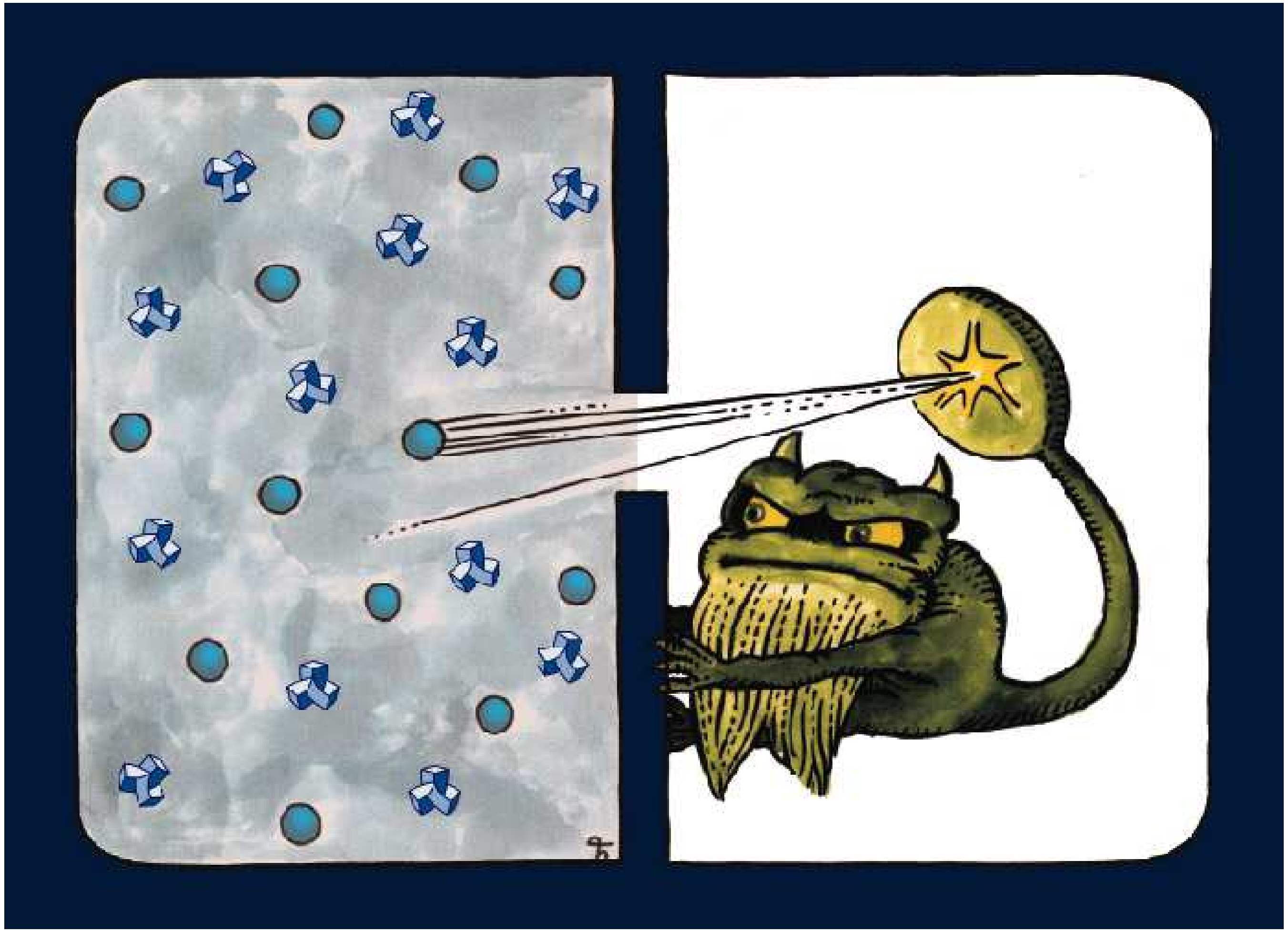
Tracks in human body I.E. water



Positron/secondary electron trajectories in water vapour



In most of those examples atomic and molecular processes served as Maxwell's demon in controlling the EEDF and spatial profiles. In Gaseous electronics /positronics some molecular processes as described by their cross sections may play the role of Maxwell's demon.



Conclusions

-New advances in measurements of the positron scattering data enable simulations,

-Swarm experiment would not be an efficient trap but it is experiment testing the limits of the present day techniques in kinetic theory for reactive gases

-A swarm experiment would provide means to normalize cross section sets. Positron swarms is a new frontier with new kinetic effects due to the non-conservative nature of the transport.

-Water vapour- positron interactions are well represented

-Important medical applications

-Efficient models of gas filled traps and possible optimization!!!

-Physical explanation of the rotating wall in single particle regime

-NOW IS THE RIGHT MOMENT TO SET UP A POSITRON MOLECULE SCATTERING DATA BASE