Evaluated electron scattering cross sections from furfural molecules for modelling particle transport in the energy range 0-10000 eV

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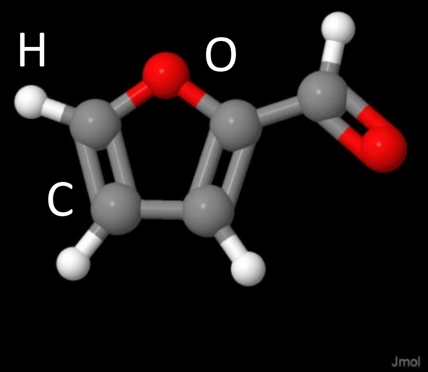
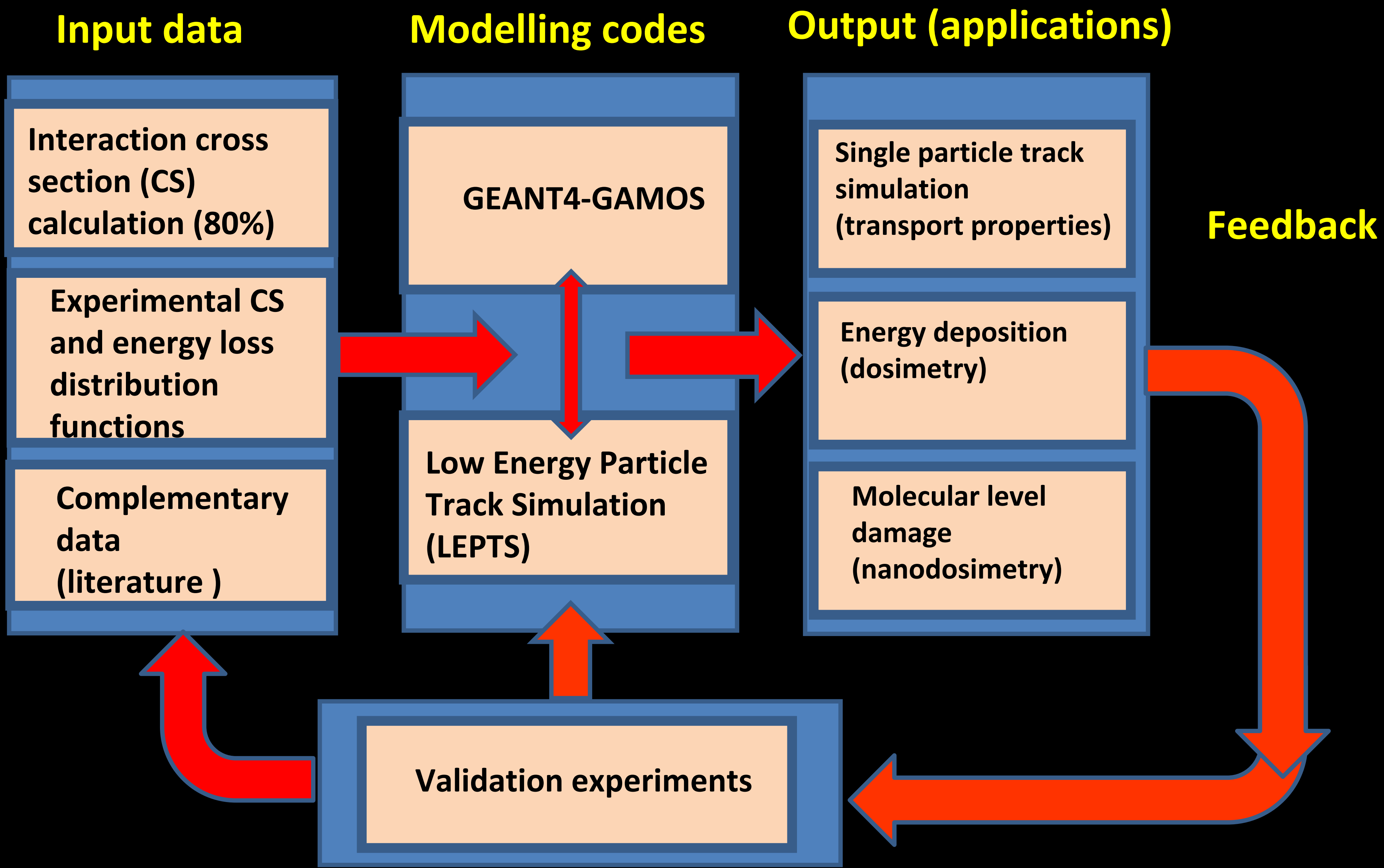
Motivation

- Biofuel precursor: atmospheric plasma or electron beam irradiation of biomass
- Analogue for the sugar backbone of the DNA helix – deoxyribose
- Improving radiation interaction models for industrial and biomedical applications

Furfural:



Modelling radiation and plama interactions



Input data bases*:

- Differential and integral, elastic and inelastic, electron scattering calculations
- Benchmarking experimental data: Elastic DCS , electronic excitation, ionisation and total scattering cross sections
- Experimental electron energy loss distribution functions
- Complementary data libraries: High energy particle interaction cross section (Born approximation)

*International collaboration

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Differential and integral, elastic and inelastic, electro

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  (Madrid)
- **Rotatior**
  Born app
- **Conden**
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e-atom, e-molecule cross sections

Differential cross section — Atomic scattering amplitud

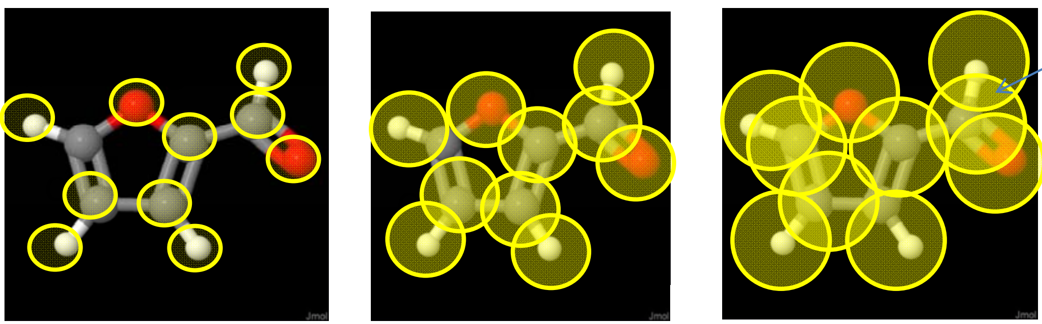
$$\frac{d\sigma^{elastic}_{molecule}}{d\Omega} = \sum_{i,j} f_i(\theta)\, f_j^*(\theta) \frac{\sin\ qr_{ij}}{qr_{ij}} = \sum_i \left| f_i(\theta) \right|^2 + \sum_{i\neq j} f_i(\theta)\, f_j^*(\theta) \frac{\sin\ qr_{ij}}{qr_{ij}}$$

Integral cross section

$$\sigma^{total}_{molecule} = \sum_{atoms} \sigma^{total}_{atom\ i} + \sigma^{interference}$$

$$\sigma^{interference} \equiv \int d\Omega \sum_{i\neq j} f_i(\theta) f_j^*(\theta) \frac{\sin\ qr_{ij}}{qr_{ij}}$$

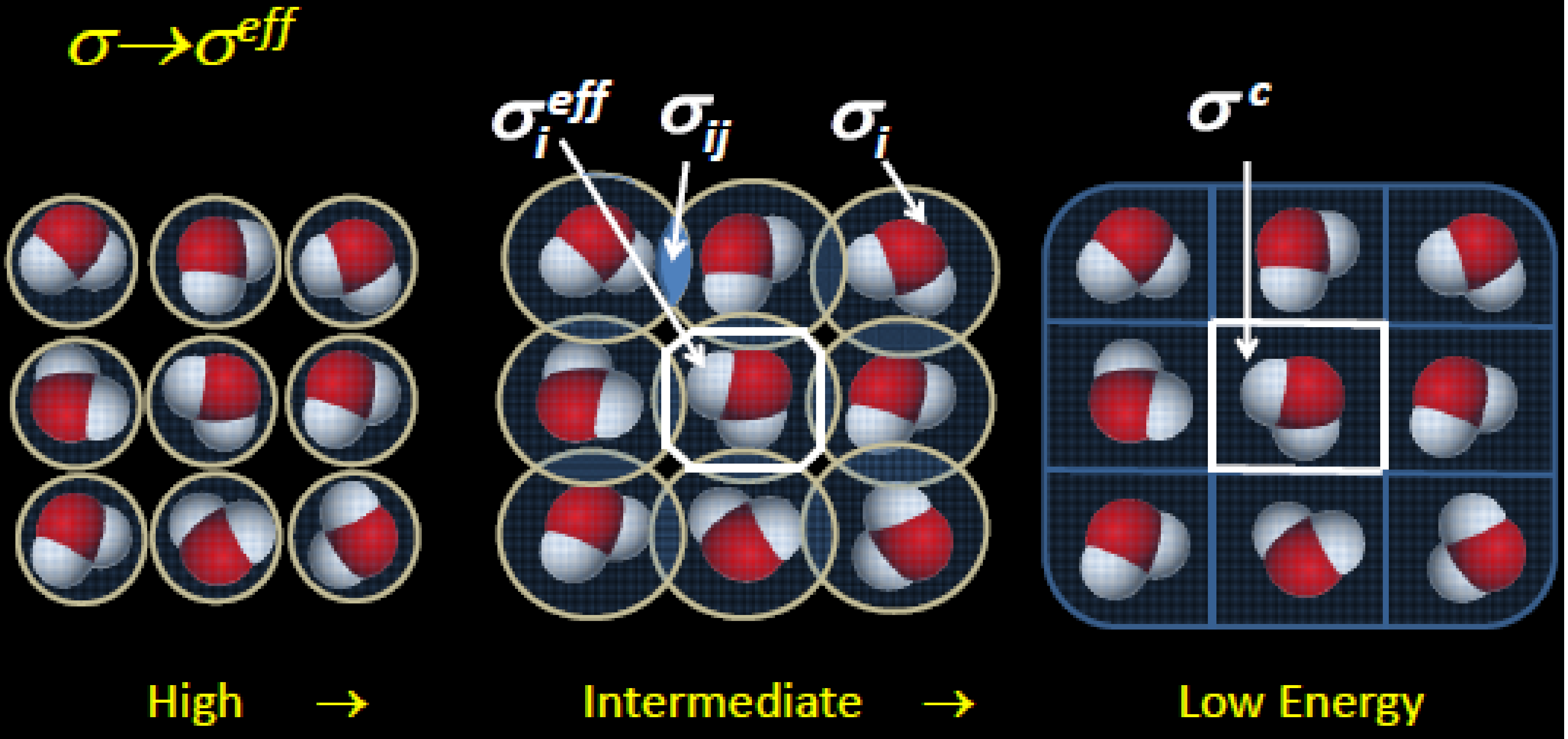
Decreasing energies →



S_{ij}
Screening coefficient

Differential and integral, elastic and inelastic, electron scattering cross section calculations

Condensed matter



Corrective factor: $s=\sigma^{eff}/\sigma=[1+(\sigma^c/\sigma)^p]^{1/p}$

P=-21→0,5% convergence

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Benchmarking experimental data

- Electron differential scattering cross sections (elastic, electronic and vibrational excitations):
  : Angular resolved crossed beam experiments (Lisbon, Adelaide)
- Ionisation and total scattering cross sections:: Transmission beam systems and mass spectrometers (Madrid, Juiz de Fora)

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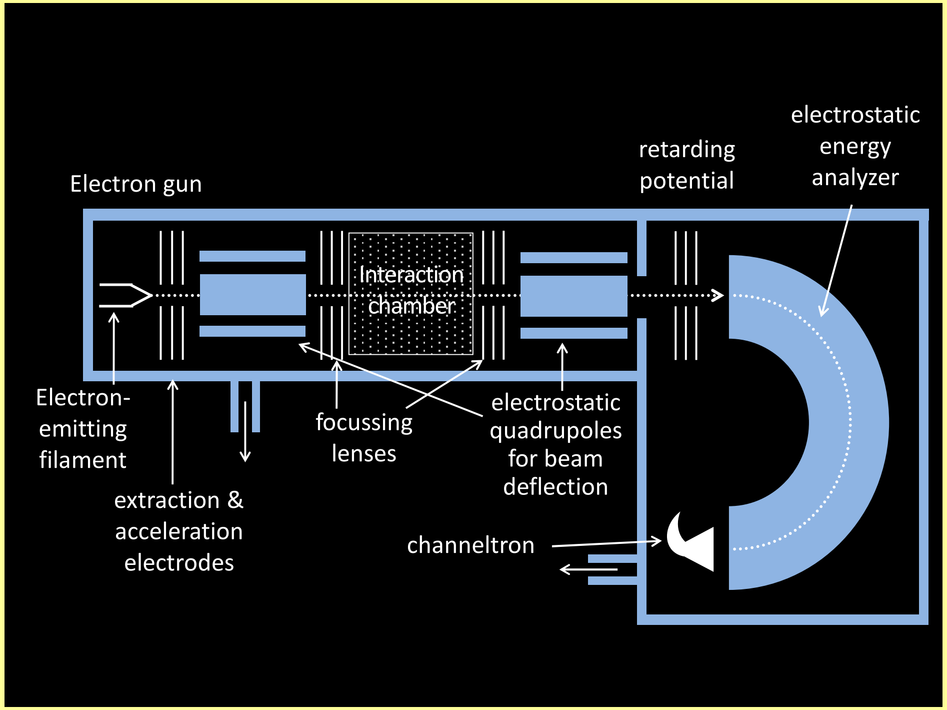
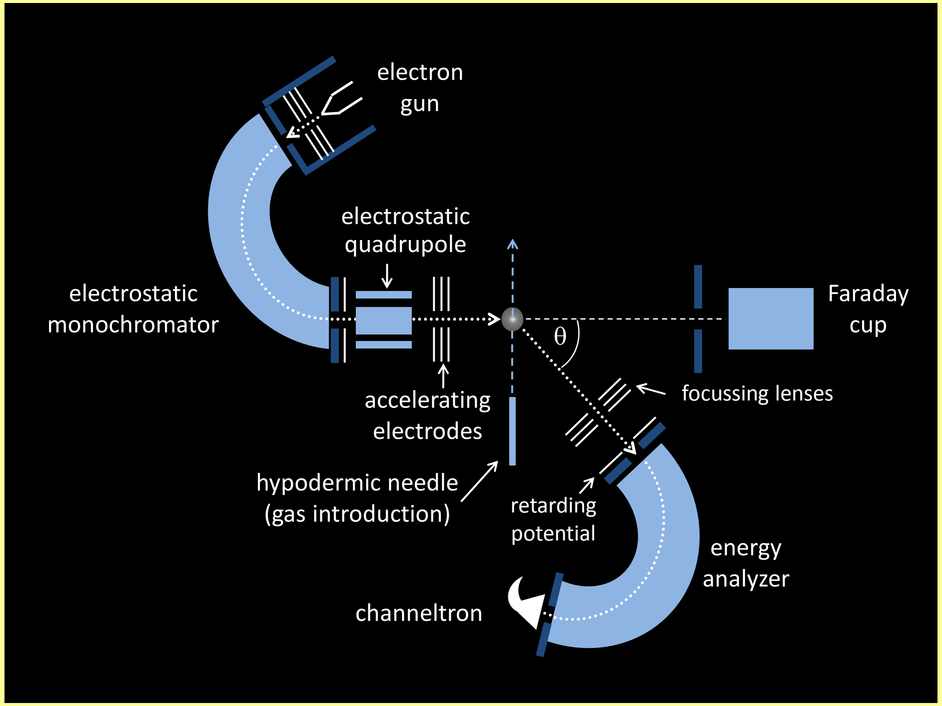
Energy loss distribution functions

Crossed beams and gas cell spectrometers (Adelaide, Madrid)

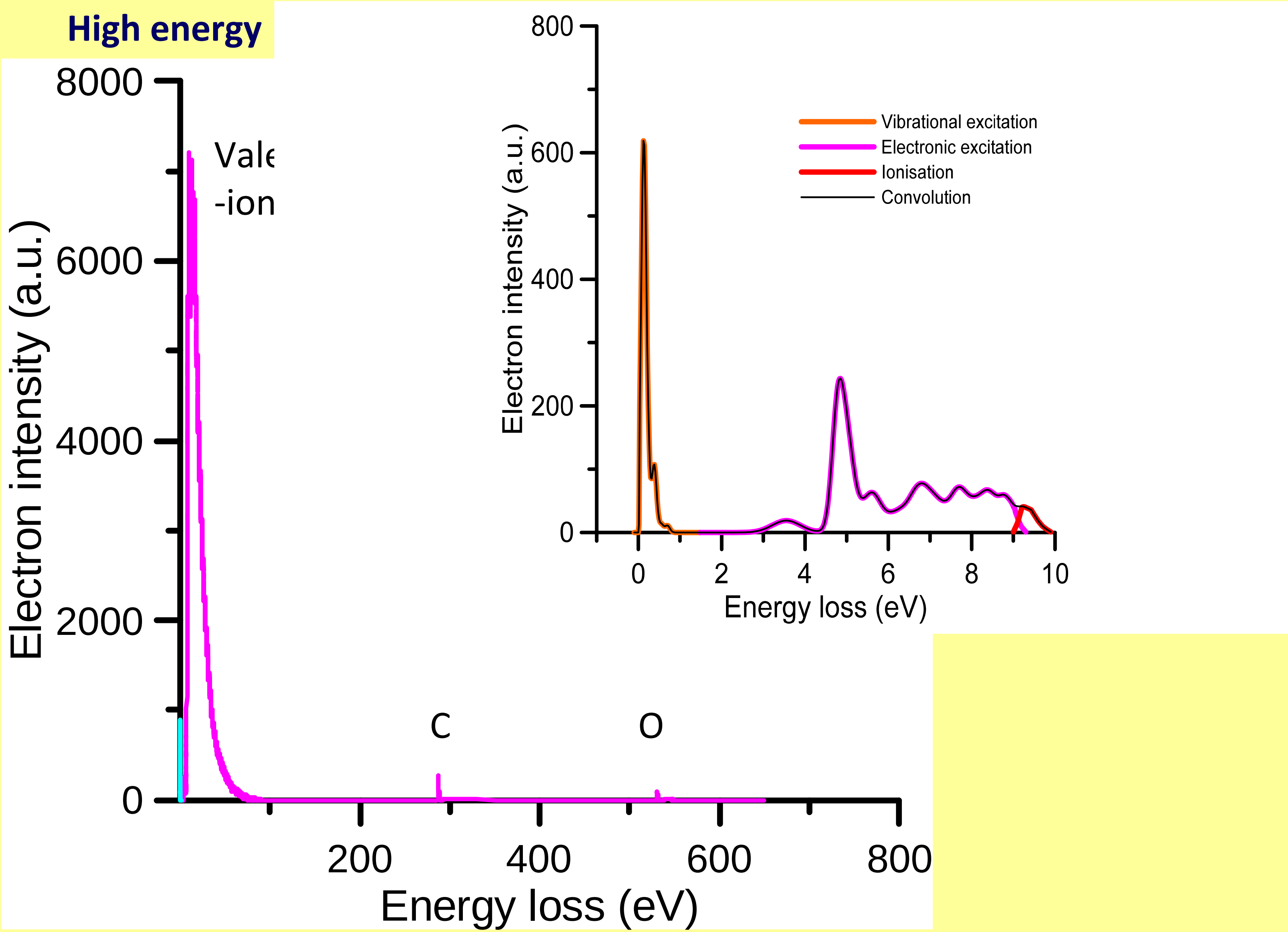




Energy loss distribution functions

Low energy

High energy



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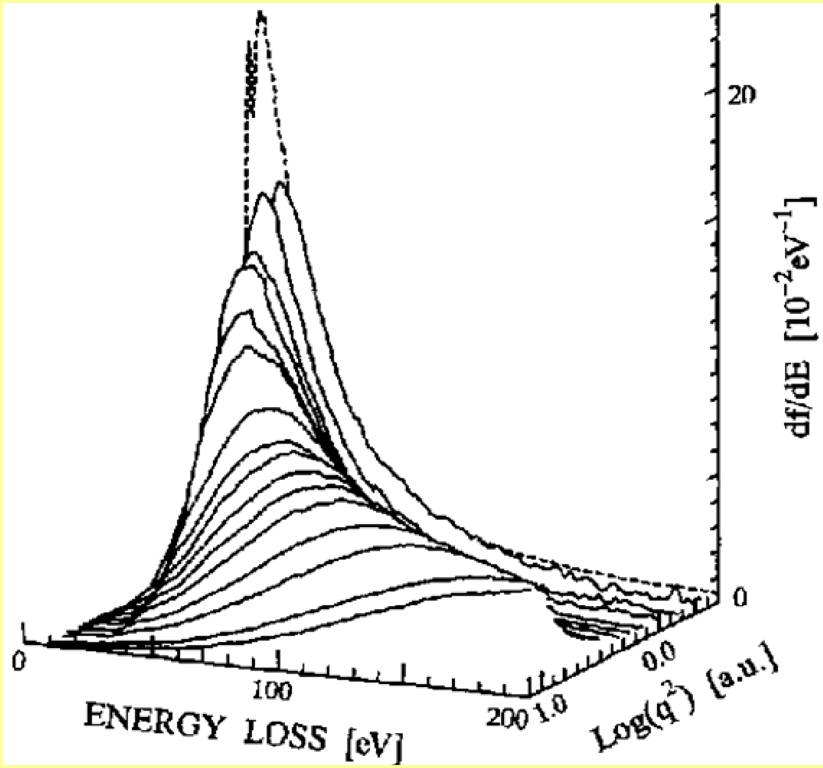
High energy electron interaction data (E>10 keV)

Molecules:

Independent atoms

$$\frac{\mathrm{d}f}{\mathrm{d}E} = F(\Delta E, q)$$

Bethe surface:

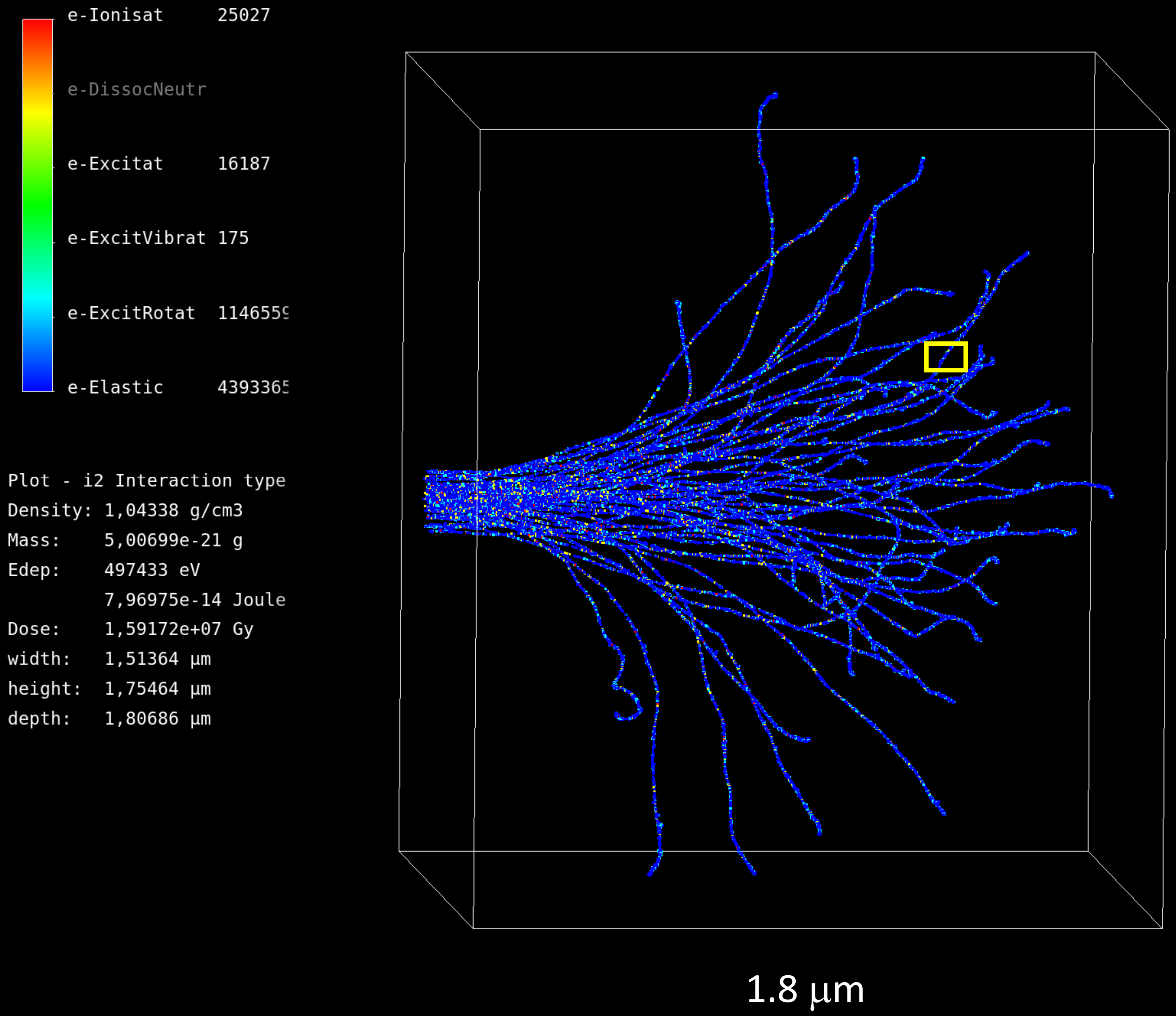


Liquid phase:

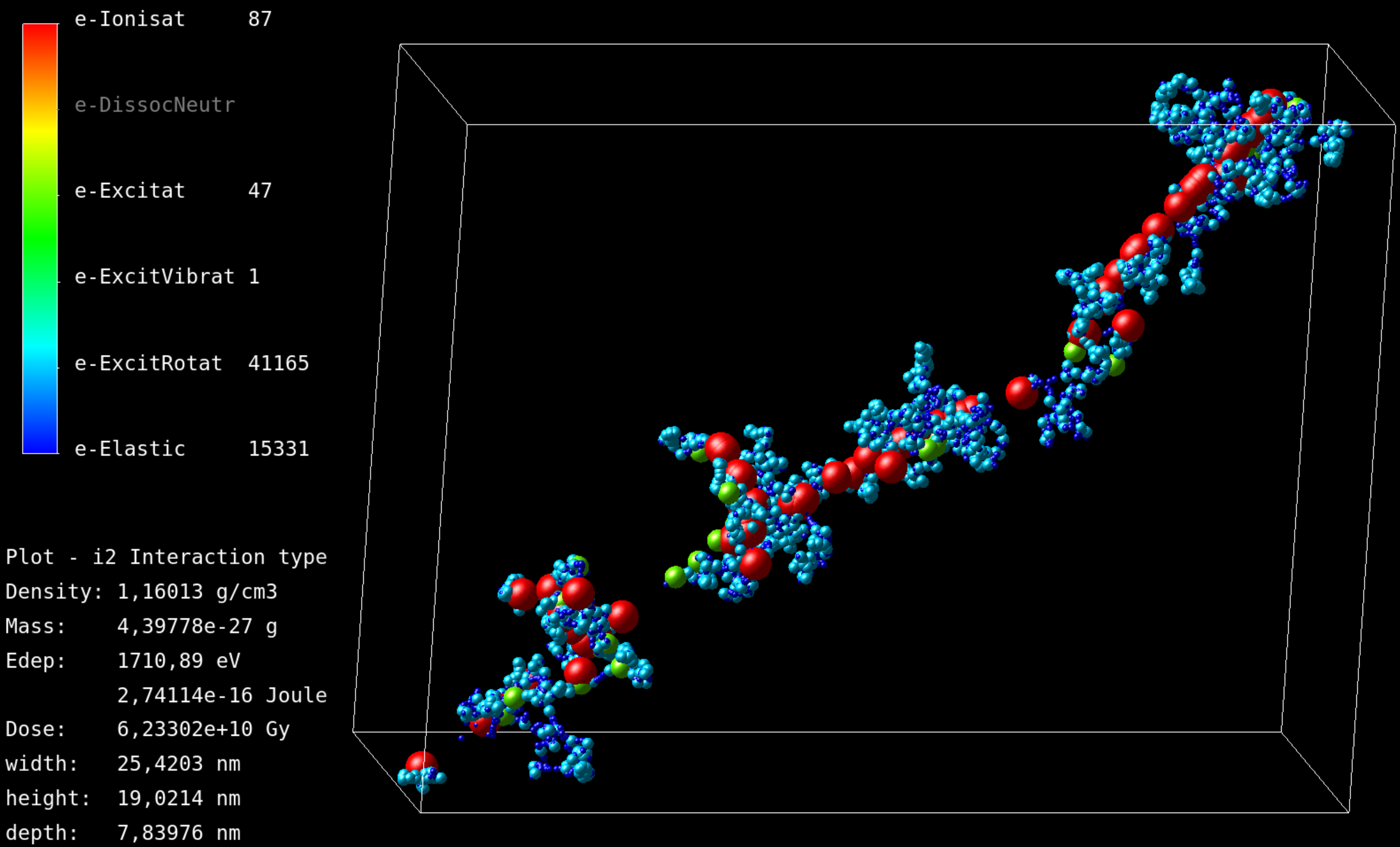
$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E\mathrm{d}q} = \frac{1}{\pi a_0 N E_0}\mathrm{Im}\left[\frac{-1}{\varepsilon(E,q)}\right]$$

Dielectric function

50, 10keV electrons through liquid furfural



Selected nanovolume



7.8 nm

Total electron scattering cross section measurements

(recent experiments at CSIC, Madrid)

- Transmission beam measurements with a double electrostatic spectrometer
- Magnetically confined electron beam attenuation measurements

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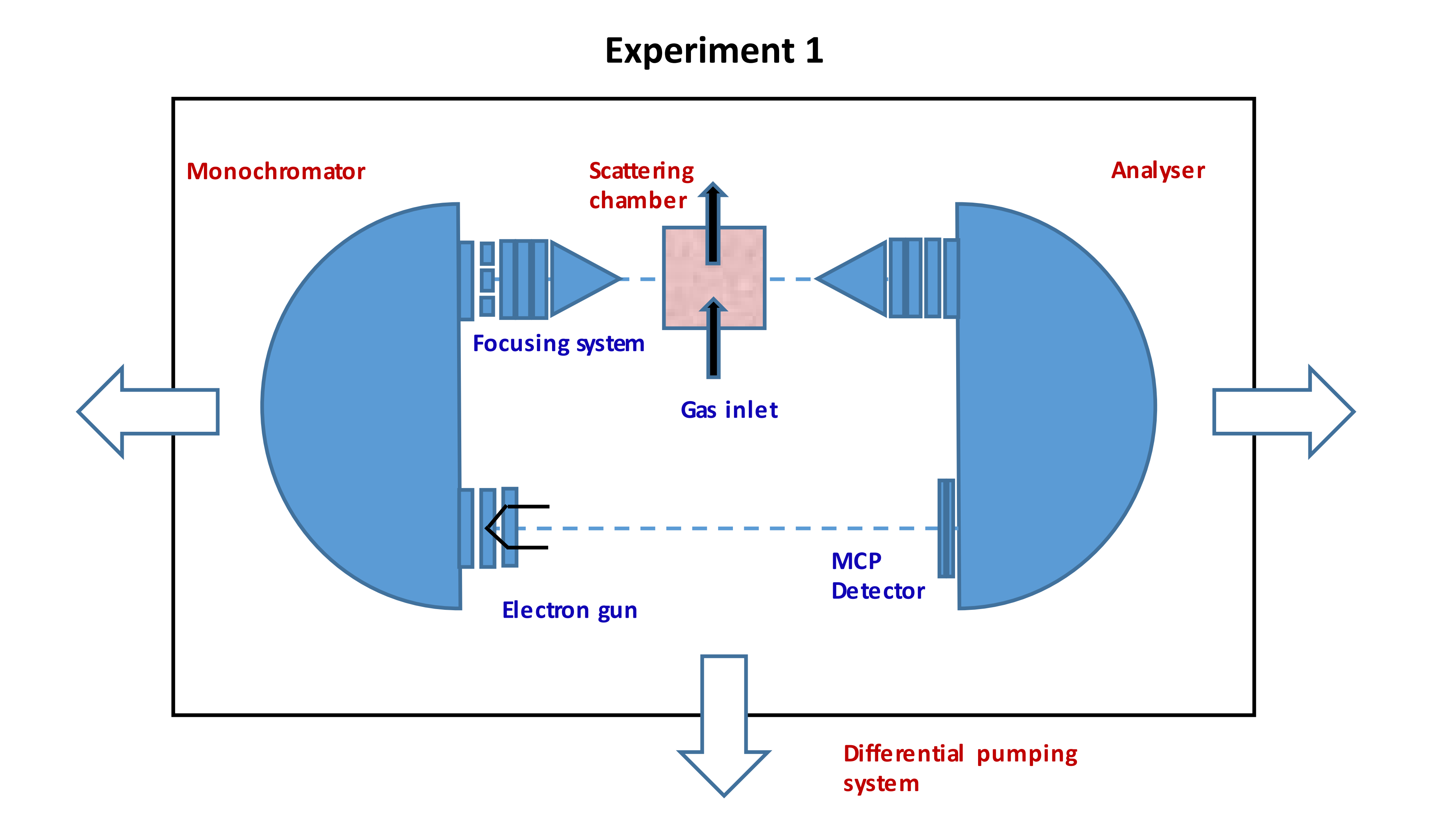

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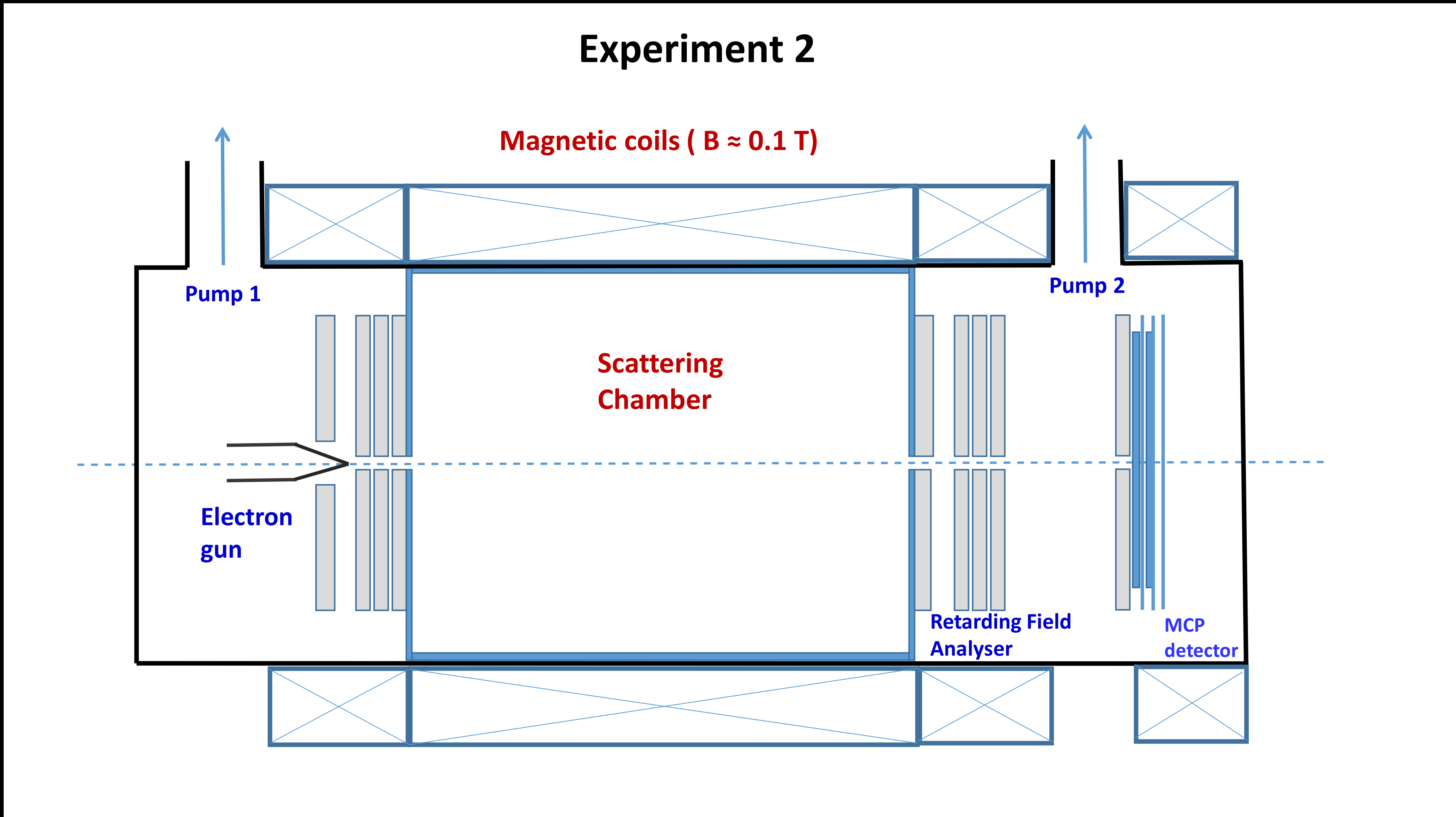
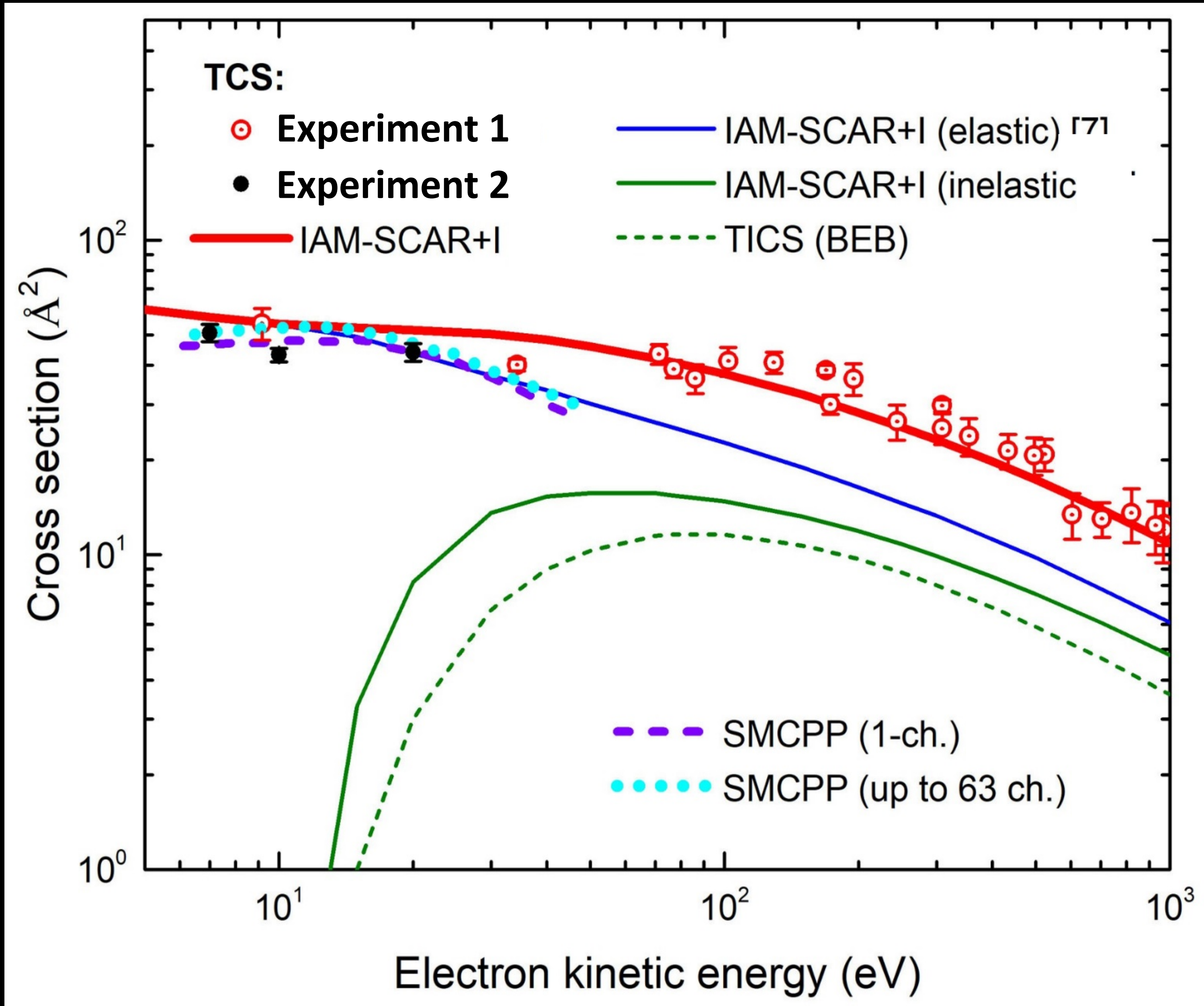
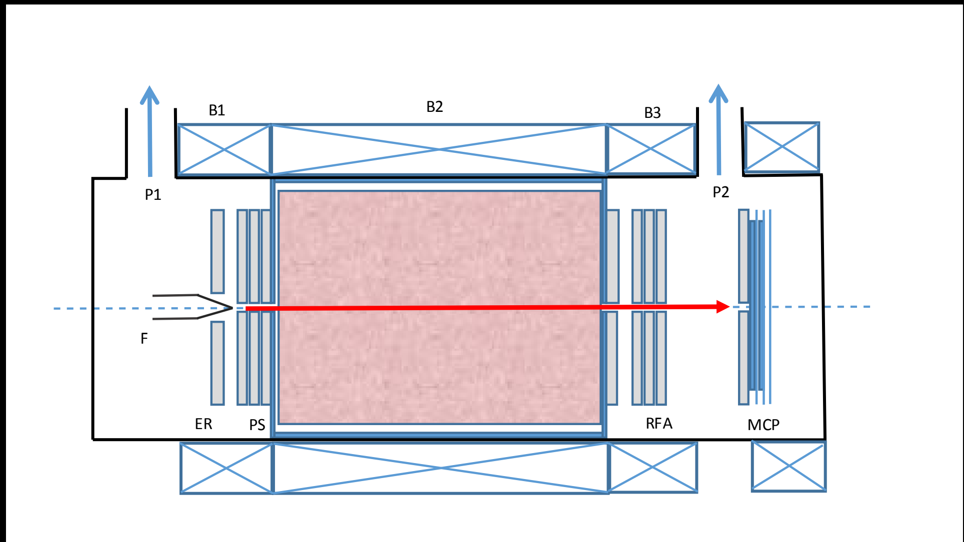


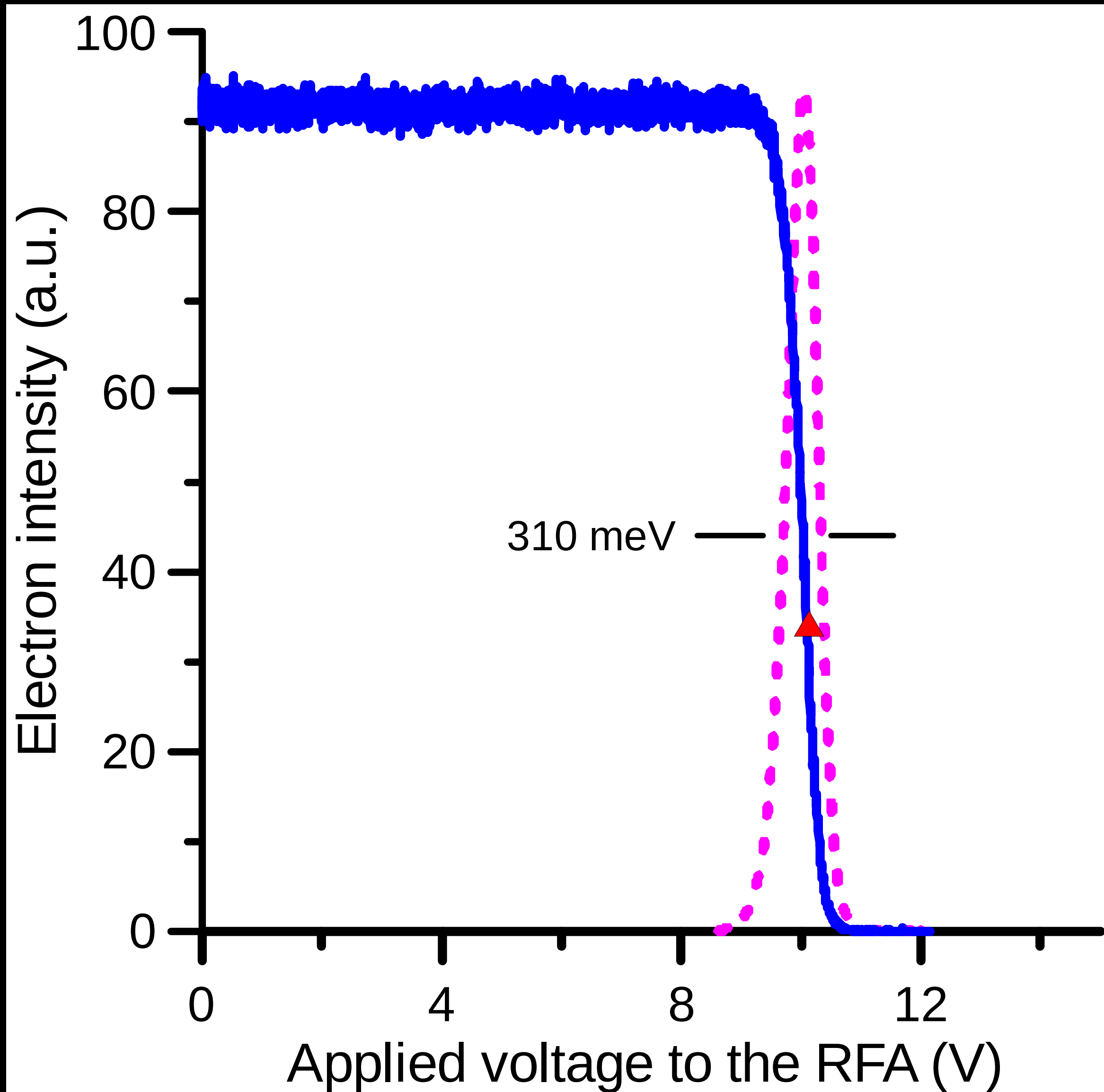
e-Furfural Total Scattering Cross Sections (TCS)



Modelling low energy electron transport in furfural under intense axial magnetic field conditions (0.1T)

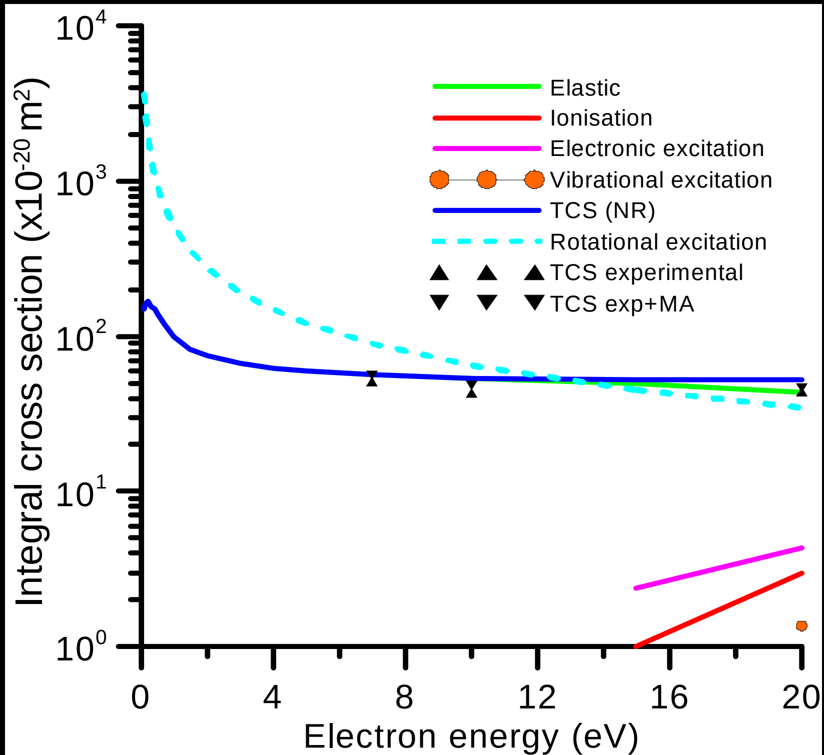


10 eV electron source

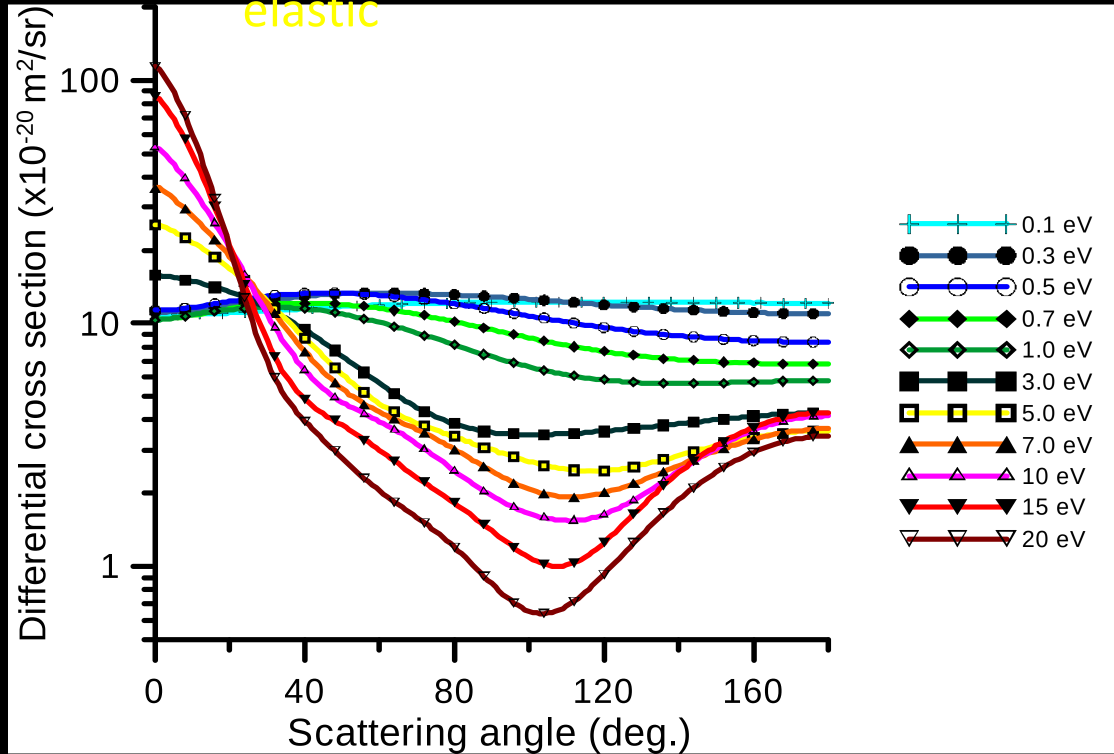


Input data

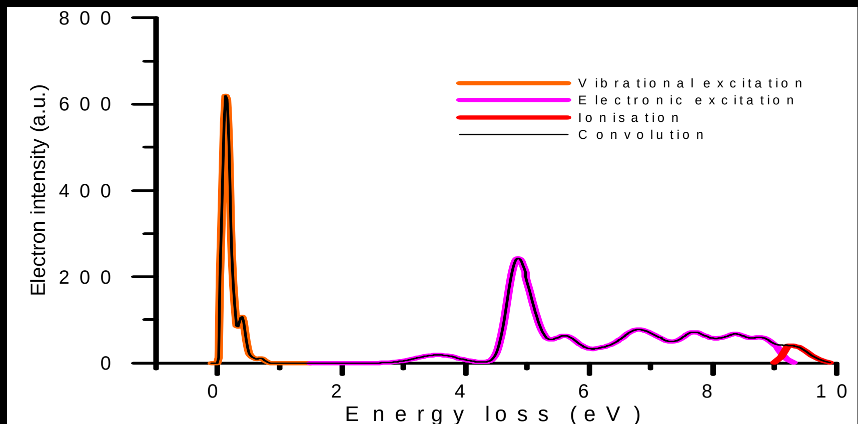
Integral



Differential elastic



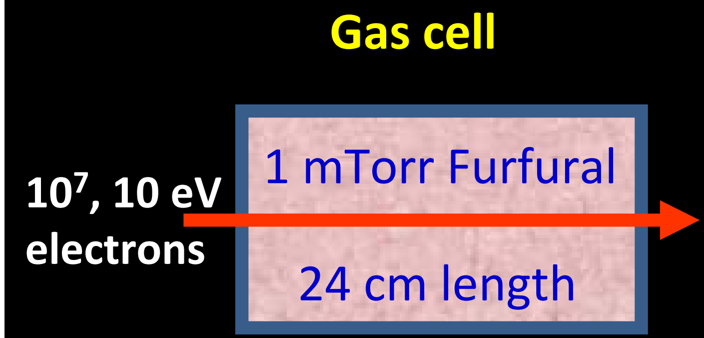
Energy loss

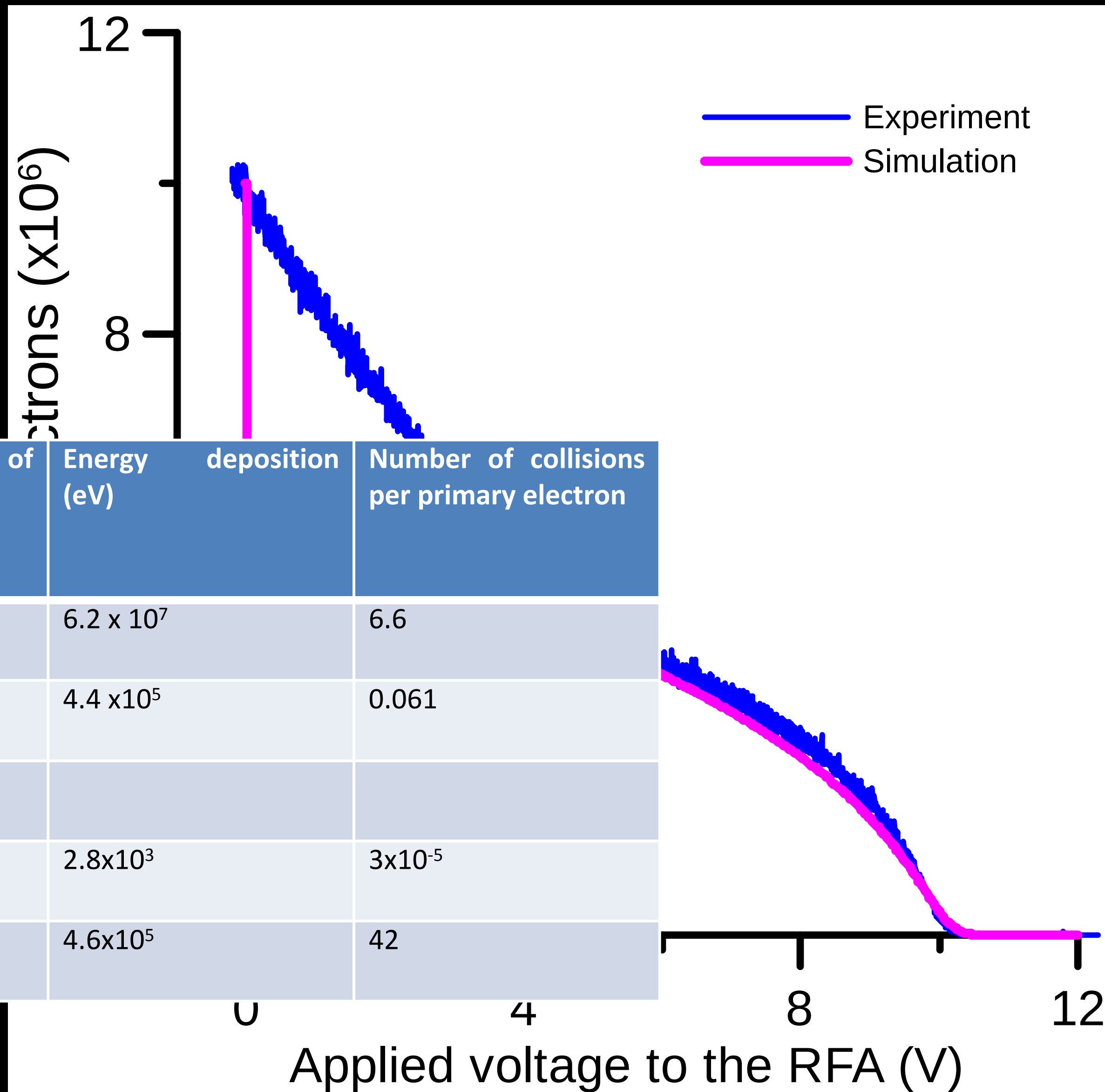


Differential Inelastic

$$\frac{d^2\sigma(E)}{d\Omega\Delta E} \propto \left(\frac{d\sigma(E)}{d\Omega}\right)_{el}^{1-\Delta E/E}$$

Transport profiles
(experimental vs simulated)





Type of interaction	Number of interactions	Energy deposition (eV)	Number of collisions per primary electron
Elastic	6.6×10^7	6.2×10^7	6.6
Electronic excitation	6.1×10^4	4.4×10^5	0.061
Vibrational excitation	-		
Ionisation	295	2.8×10^3	3×10^{-5}
Rotational excitation	4.2×10^8	4.6×10^5	42

Conclusions

- An evaluated database for e-furfural interactions has been obtained through an international collaboration
- The Low Energy Particle Track Simulation (LEPTS) code provides molecular level information for biomedical and industrial applications (using the above data)
- Accurate total electron scattering cross sections are reference values to check data base consistency (new experimental systems have been presented)
- Validation experiments provide valuable information on further improvements in both input data and experimental techniques

Acknowledgements

- M. J. Brunger, D. B. Jones
- P. Limão-Vieira, F. Ferreira da Silva

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