Evaluated electron and positron-molecule scattering data for modelling particle transport in the energy range 0-10000 eV

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Modelling tools for molecular data validation

- High energy ($E > 10$ keV) primary radiation (photons, electrons and ions): GEometry ANd Tracking4 (GEANT4)
- Low energy ($E < 10$ keV) secondary particles (electrons, positrons and radicals): Low Energy Particle Track Simulation (LEPTS)
Modelling procedure to validate interaction data in molecular media

- Interaction cross section data
- Energy loss distribution functions
- Angular distribution functions
- Source geometry and emission spectra
- LEPTS Code
- Laboratory verification
- General MC Programme GEANT4
- GAMOS Architecture
Input data

• High energy photons and ions:
  (Literature: Evaluated Data Bases)

• High energy (>10keV) electrons/positrons:
  (First Born approximation- Bethe surfaces)

• Low energy electron, positrons and radicals:
  (Evaluated theoretical and experimental data-EPEDAT)
Electron and positron evaluated data EPEDAT

• **Experimental sources:**
  – Electron and positron scattering with molecules: CSIC, Flinders University (FU), Universidade Nova de Lisboa (UNL), Sophia University (SU), Australian National University (ANU)
  – Electron transfer to molecules: CSIC, New University of Lisbon (UNL)

• **Theoretical methods:**
  – Electron and positron scattering with molecules: CSIC (IAM-SCAR), Open University (R-matrix), University of Innsbruck (Single-Centre Expansion)
Beam-gas experiments-1

Total cross sections (5-7%)
Ionisation cross section (7-10%)
Partial ionisation (10-20%)
Neutral dissociation (25-40%)
Energy loss (forward dir.) (10%)
Beam-gas experiments-2

e/p magnetically confined beam

Differential and integral cross section measurements

Magnetic coils (0.2 T)

p-Source

Frozen Ne Moderator

Gas cooling chamber

Scattering chamber

RPA

MCP

ANU-Canberra (p)      CSIC-Madrid (e)
Crossed-beam experiments

- Elastic: (10-20%)
- Inelastic: (20-40%)
- Energy loss (angular): (10-20%)

Molecular beam

FU-Adelaide
UL-Liège
SU-Tokyo
Crossed-beam experiments-2

electron transfer induced dissociation

No absolute cross section values

CSIC-Madrid
UNL-Lisbon
Calculations
Electron and positron scattering in molecular and condensed media

• **Atoms:** Model potential representation,

• **Molecules:**
  – Independent atom model (IAM), Aditivity rule (AR) with screening corrections (SCAR) and interference terms
  – Additional dipole rotational excitations (FBA)

• **Condensation effects:** Atomic and molecular clusters, liquids, solids (IAM-SCAR)

• **Low energy (< 20 eV) extension:** Single-Centre Expansion and R-Matrix procedures
Atoms

Electrons: \( V(r) = V_{st}(r) + V_{ex}(r) + V_{pol}(r) + i[V_{abs}(r)] \)

Positrons: \( V(r) = V_{st}(r) + V_{pol}(r) + i[V_{abs}(r) + V_{ps}(r)] \)
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Molecules

Differential cross sections

\[
\frac{d\sigma_{\text{elastic molecule}}}{d\Omega} = \sum_{i,j} f_i(\theta)f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}} = \sum_i |f_i(\theta)|^2 + \sum_{i \neq j} f_i(\theta)f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}}
\]

Integral cross sections

\[
\sigma_{\text{total molecule}} = \sum_{\text{atoms}} \sigma_{\text{total atomi}} + \sigma_{\text{interference}}
\]

\[
\sigma_{\text{interference}} \equiv \int d\Omega \sum_{i \neq j} f_i(\theta)f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}}
\]
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Condensed matter

σ \rightarrow σ^{eff}

High \rightarrow \text{Intermediate} \rightarrow \text{Low Energy}

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

P = -21 \rightarrow 0.5\% convergence
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IAM-SCAR water

(H₂O)₃ cluster

Liquid water

H₂O molecule

e⁻, e⁺-track
Some examples of calculations

Differential elastic scattering cross sections $e$-$\text{GeF}_4$

- Experimental data from H. Tanaka (SU Tokyo)
- IAM-SCAR calculation
Some examples of calculations

Total electron scattering cross sections

e-CH₄

[Graph showing total scattering cross sections for different energies with various data points and labels.]
Example of input data

Three main classes of input data are needed:

1. Scattering CS
2. Energy loss distrib. functions
3. Angular distrib. functions

Uncertainties:  
1. Scattering CS: 5-20%
2. Energy loss distrib. functions: 10-20%
3. Angular distrib. functions: 10-20%
Integral CS: 0.1 eV – 10 keV

1. Scattering CS

- Total scattering CS (5-7%)
- Integral CS for:
  - elastic scattering (10-15%)  
  - Ionization (7-10%)  
  - electronic excitation (20%)  
  - vibrational excit. (20%)  
  - rotational excit. (10-15%)  
  - neutral dissociation (25%)  
  - DEA (10-15%)  
  - self-consistency:  
    \[ \Sigma \text{int. CS} = \text{total CS} \]
- CS table is compiled from typically \( \sim 15 \) different sources!

example: methane
Differential CS 0° -180°

3. Angular distrib. functions

- Elastic DCS
  - Tabulated values from 0° to 180° on a 1° grid from ~6 sources
  - Data from experimental sources are extrapolated towards 0° and 180°

- Inelastic DCS
  - Aim: tabulated form, 0°-180°
  - Present source: approximation by empirical formula

\[
\frac{d^2 \sigma(E)}{d \Omega d \Delta E} \propto \left( \frac{d \sigma(E)}{d \Omega} \right)_{el}^{1 - \Delta E/E}
\]
e-Furfural
Energy loss distribution function

Electron intensity (a. u.)

Energy loss (eV)

- Vibrational
- Electronic
- Ionisation

O
N
Current state of the Madrid data collection

Molecules currently included:
- Water (e, p)
- Argon (e, p)
- Nitrogen, Oxygen (e, p)
- Methane (e)
- Ethylene (e)
- Tetrahydrofuran (e)
- Sulphur hexafluoride (e)
- Pyrimidine (e, p)
- Furfural (e)

Processes currently included:
- elastic scattering
- ionization, Auger e- generation
- vibrational and rotational excitation (average of existing states)
- electronic excitation (all states according to EEL spectra)
- neutral dissociation
- dissociative electron attachment
- positronium formation
- annihilation
Example: 10keV electrons through furfural

Plot - i2 Interaction type
Density: 1,16013 g/cm³
Mass: 4,39778e-27 g
Edep: 1710.89 eV
2.74114e-16 Joule
Dose: 6.23302e+10 Gy
width: 25,4203 nm
height: 19,0214 nm
depth: 7,83976 nm
Importance of energy loss uncertainties

Energy Deposition under different inner shell conditions

- Inner Shell included
- IS increased 20%
- No inner shell - only valence
Importance of elastic scattering

Energy Deposition under isotropic elastic scattering conditions

- Inner Shell included
- IS increased 20%
- No inner shell - only valence
- Isotropic DCS <3keV

Depth (microns)

Energy deposition (eV)
Particle transport data evaluation:
20 eV magnetically confined electrons transmitted through 140 mm length gas (3 mTorr furfural pressure) cell
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20 eV magnetically confined electrons transmitted through 140 mm length gas (3 mTorr furfural pressure) cell

Low angle DCS uncertainties

Rotational cooling and high angle DCS
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