Geant4-DNA datasets for ionization and excitation of liquid water by protons above 100 MeV

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26th Geant4 Collaboration Meeting

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Outline

- Motivation and goal
- RPWBA theory
- Liquid water GOS
- Datasets calculation
- Implementation
- Validation
- Implementation verification

Motivation and goal

http://geant4-dna.in2p3.fr/

PROTONS (named "proton") **Liquid water**

Max. energy Limit → 100 MeV

Max. energy of clinical proton therapy beams → ≈250 MeV

Range in liquid water → ≈ 39 cm

- **Nuclear scattering** : G4DNAElastic
  - G4DNAIonElasticModel
    - applicable energy range : 100 eV - 1 MeV
    - cut at 100 eV (5)
    - type : interpolated
    - Geant4-DNA physics constructors : default, option2, option4, option6

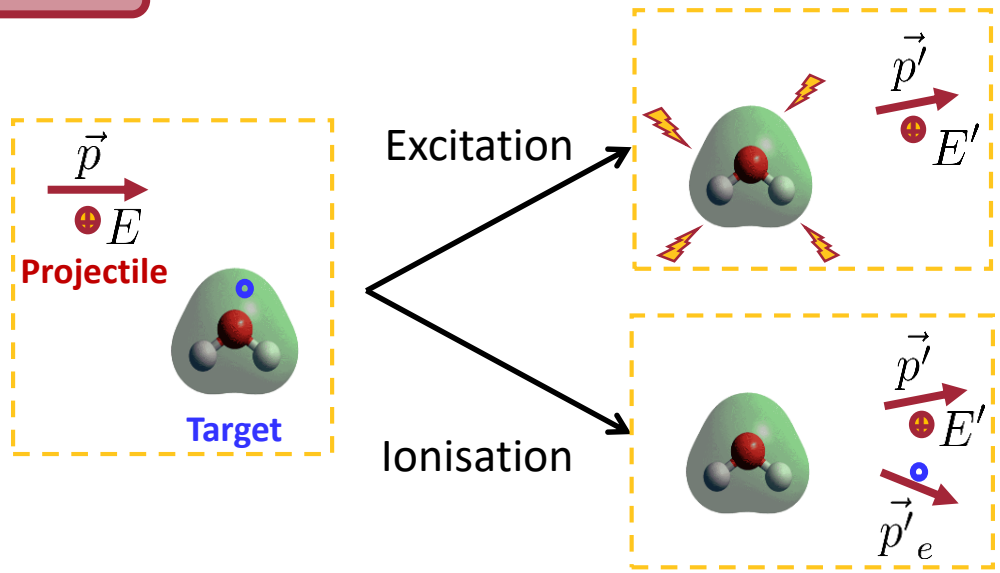
- **Electronic excitation** : G4DNAExcitation
  - G4DNAMillerGreenExcitationModel
    - applicable energy range : 10 eV - 500 keV
    - type : analytical
    - constructors : default, option2, option4, option6
  - G4DNABornExcitationModel (3)
    - applicable energy range : 500 keV - 100 MeV
    - type : interpolated
    - constructors : default, option2, option4, option6

- **Ionisation** G4DNAIonisation
  - G4DNARuddIonisationModel (G4DNARuddIonisationExtendedModel is also usable, °)
    - applicable energy range : 0 eV - 500 keV
    - cut at 100 eV (5)
    - type : interpolated
    - constructors : default, option2 (°), option4, option6
  - G4DNABornIonisationModel
    - applicable energy range : 500 keV - 100 MeV
    - type : interpolated
    - constructors : default, option2, option4, option6

- **Electron capture** : G4DNAChargeDecrease
  - G4DNADingfelderChargeDecreaseModel
    - applicable energy range : 100 eV - 100 MeV
    - type : analytical
    - constructors : default, option2, option4, option6

RPWBA theory

RPWBA **Relativistic Plane Wave Born Approximation**



Individual inelastic collisions

In terms of

Energy loss $W = E - E'$

Momentum transfer $\vec{q} = \vec{p} - \vec{p'}$

Recoil energy Q

DDCS **Doubly differential cross section**

$$\frac{d^2\sigma}{dW\,dQ} = \frac{2\pi Z_P^2 e^4}{m_e c^2 \beta^2}\left\{\frac{2m_e c^2}{WQ(Q+2m_e c^2)} + \frac{2m_e c^2}{[Q(Q+2m_e c^2) - W^2]^2}\left[\beta^2 - \frac{W^2}{Q(Q+2m_e c^2)}\right]\right\}\frac{df(Q,W)}{dW}$$

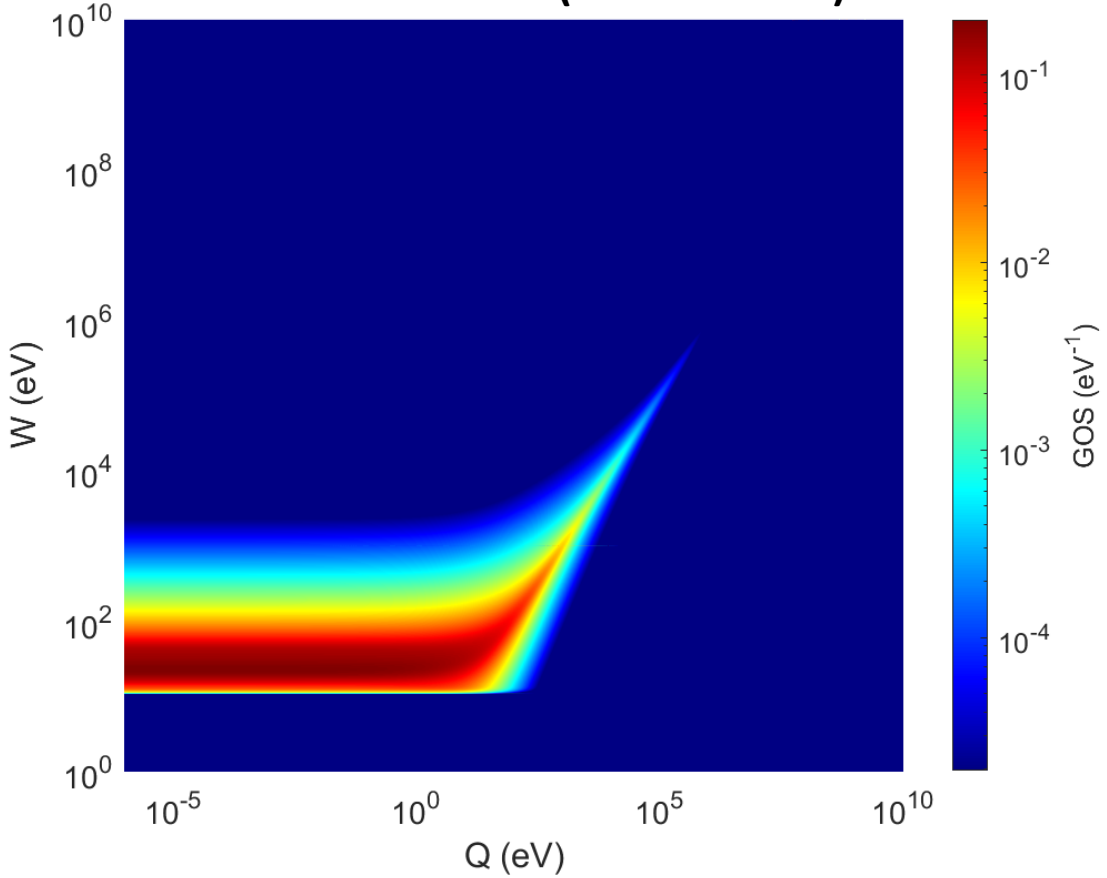
Generalized oscillator strength (GOS)

Response of the material $\frac{df(Q,W)}{dW}$

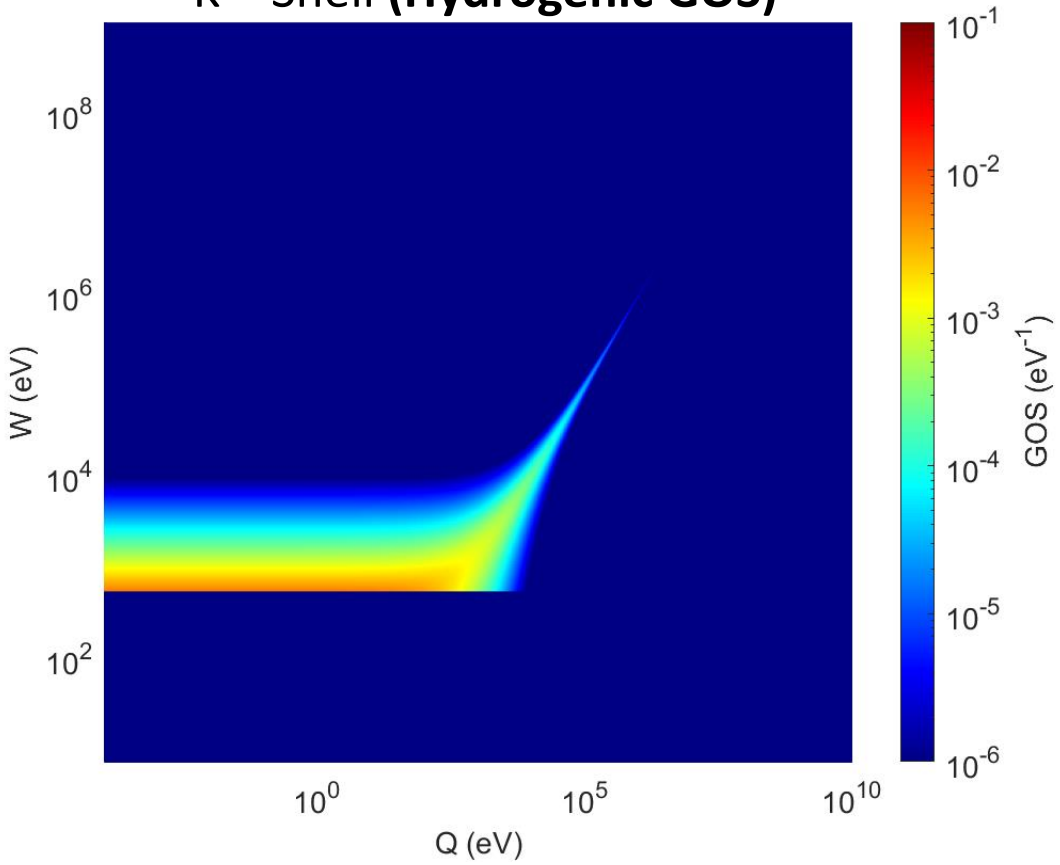
Liquid water GOS

Ionisation GOS

Sum of outer shells **(Drude model)**



K – Shell **(Hydrogenic GOS)**

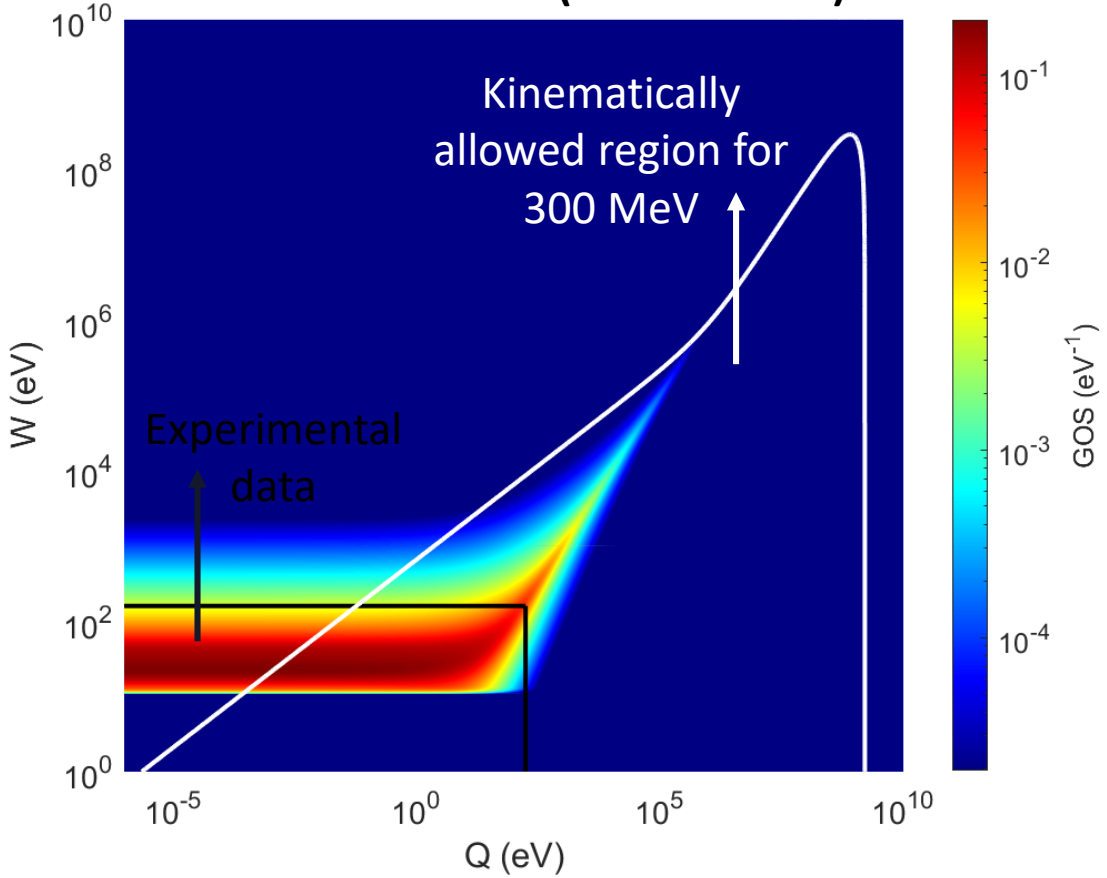


Parameters values taken from [D. Emfietzoglou / *Radiation Research 164 (2005) 202–211]*

Liquid water GOS

Ionisation GOS

Sum of outer shells **(Drude model)**



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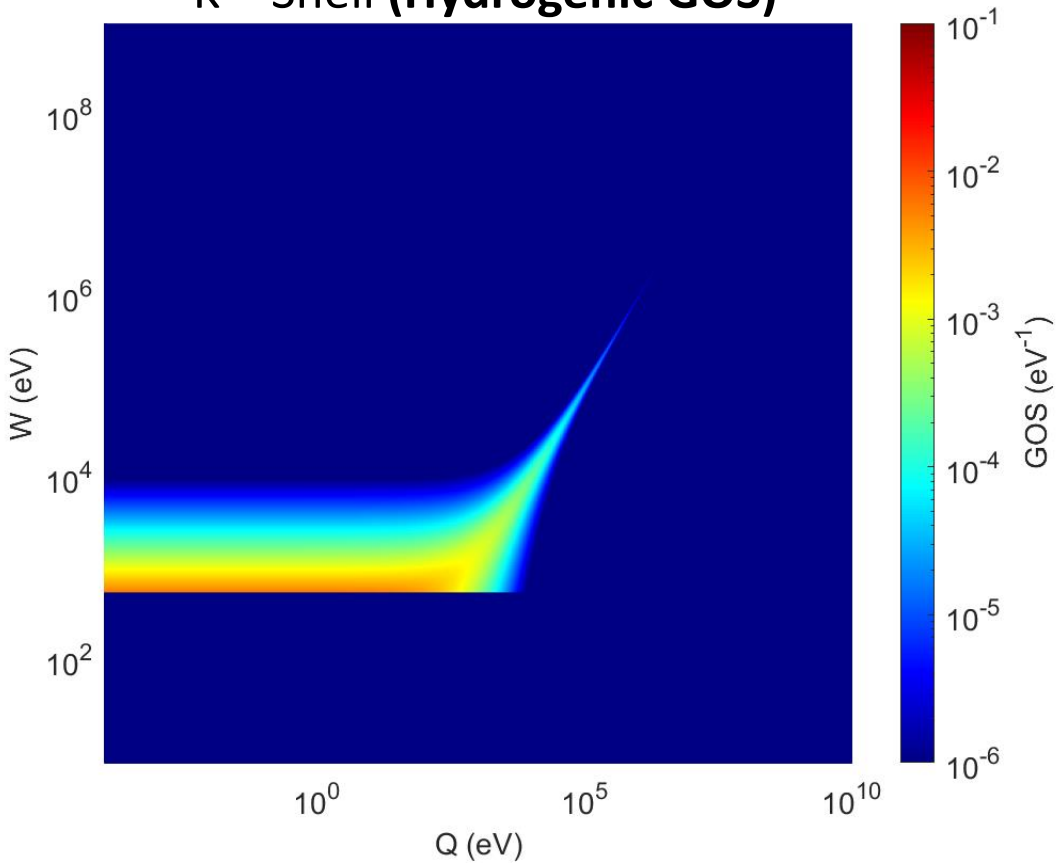

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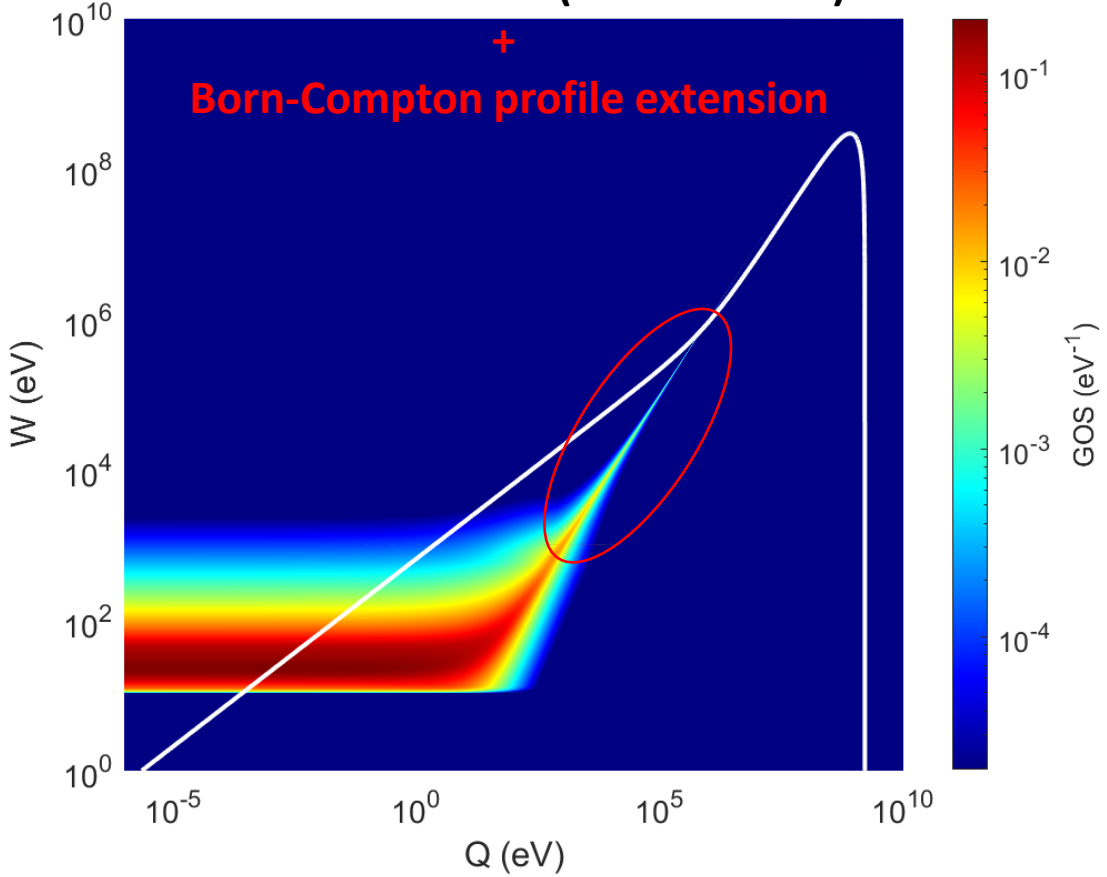
Liquid water GOS

Ionisation GOS

Sum of outer shells **(Drude model)**

+

Born-Compton profile extension



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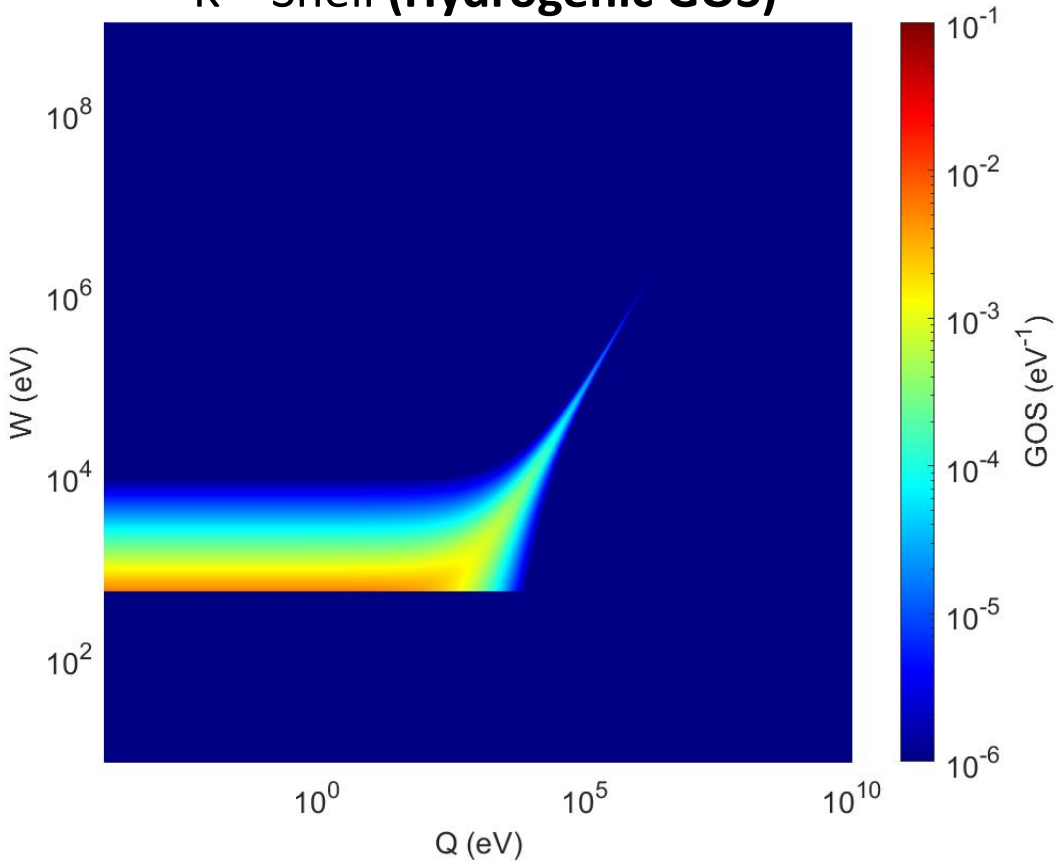

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Liquid water GOS

Ionisation GOS

Sum of outer shells **(Drude model)**
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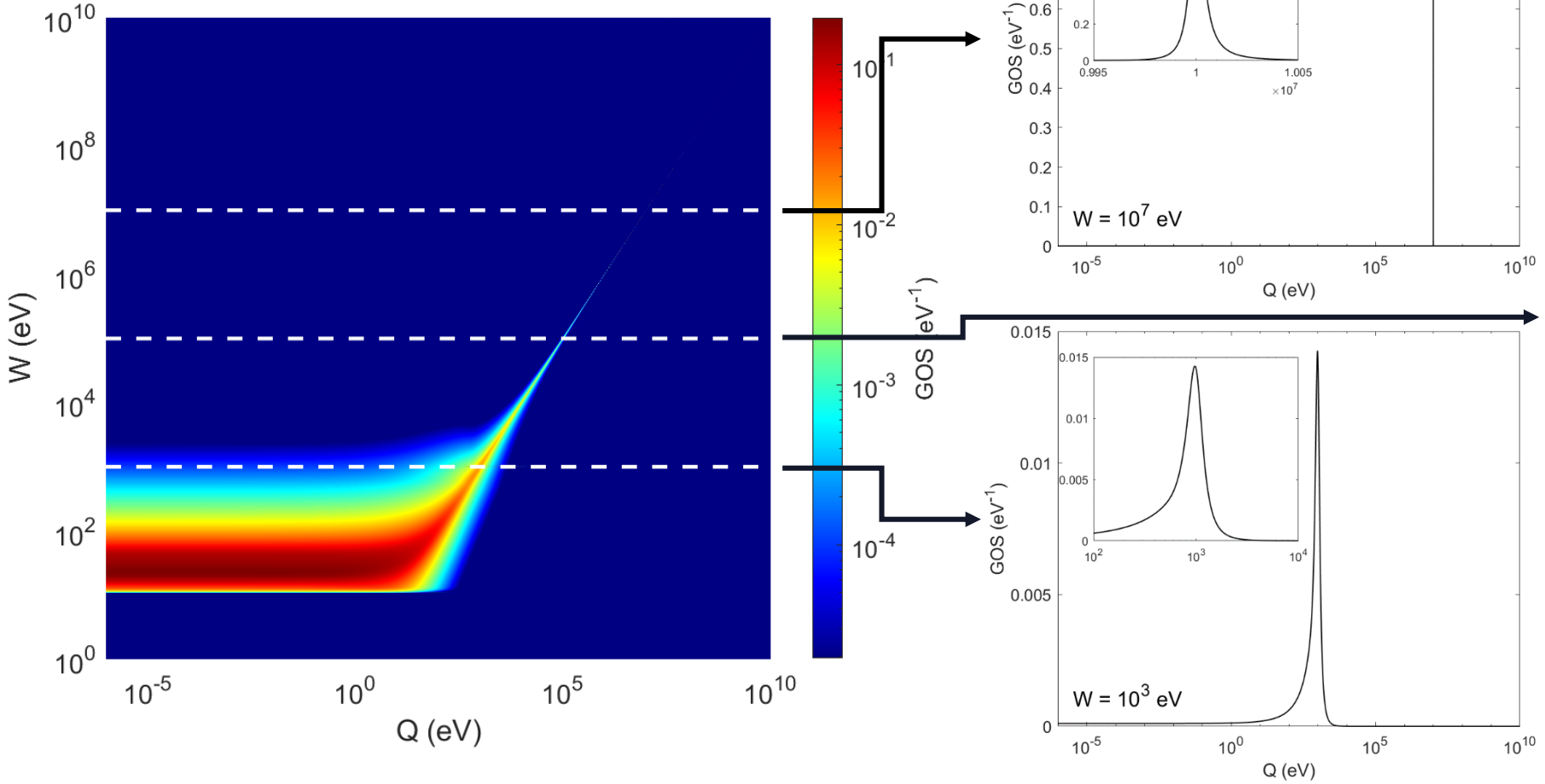
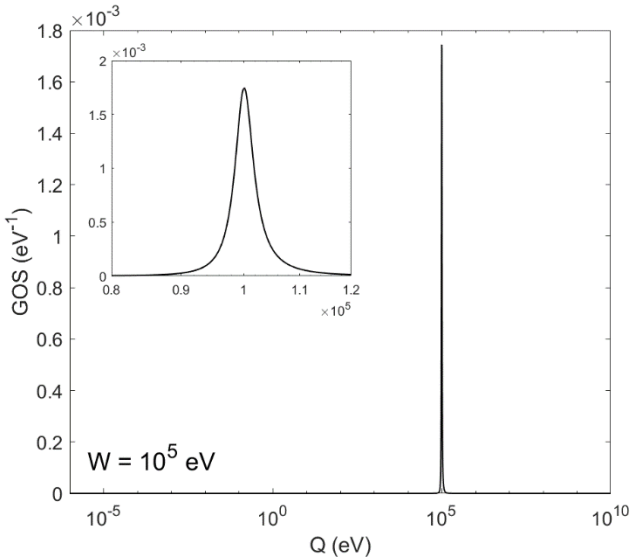


Adaptative grid to reproduce numerically the Bethe-Ridge accurately

Necessary for numerical integration of DDCS

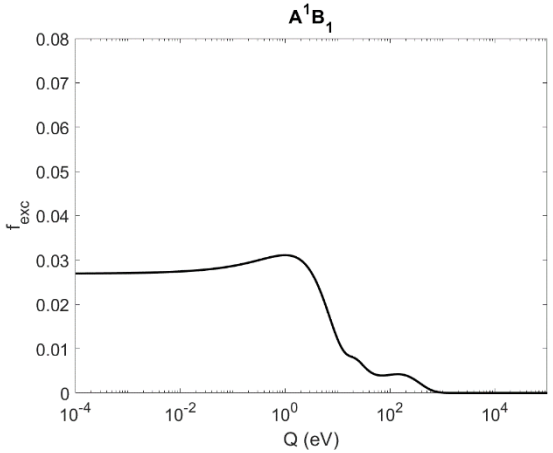


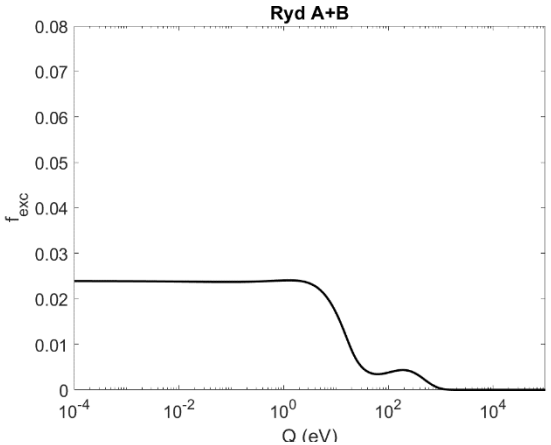
Liquid water GOS

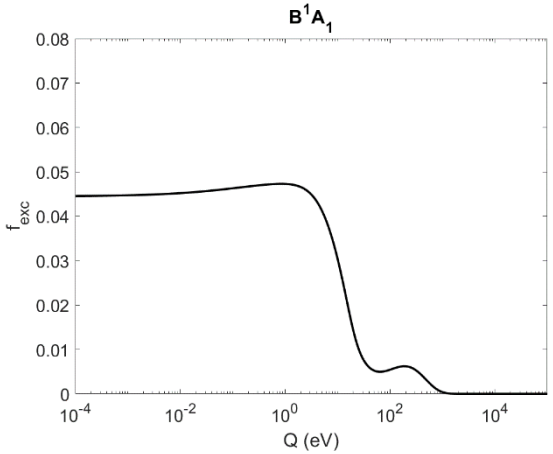
Excitation GOS

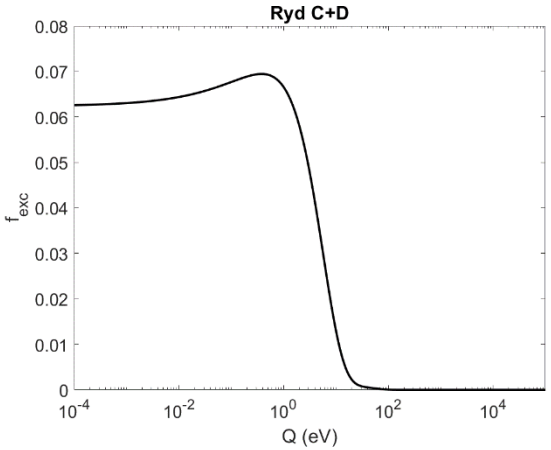
$$\frac{df_{\mathrm{exc}}(Q,W)}{dW} = f_{\mathrm{exc}}(Q)\delta(W - W_{\mathrm{exc}})$$

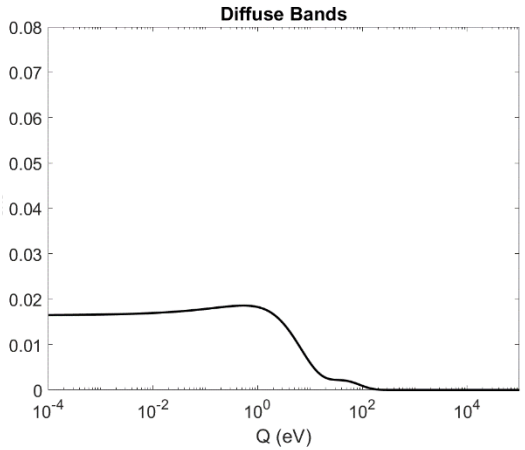
Discrete transitions











Transition	Discrete energy (eV)
(A^1B_1)	8.10
(B^1A_1)	10.10
(Ryd A+B)	12.00
(Ryd C+D)	13.51
(Diffuse bands)	14.41

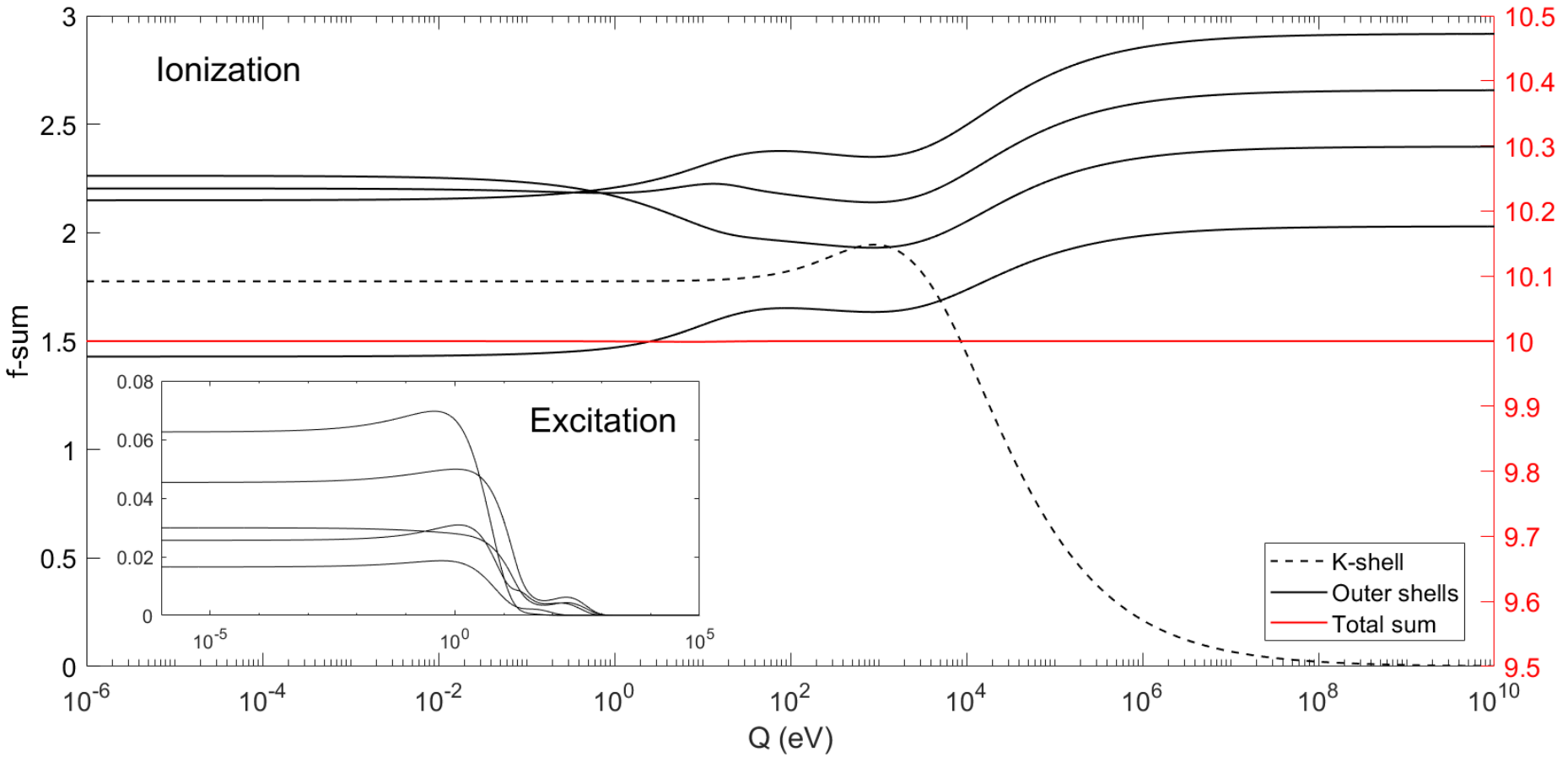
Parameters values taken from

[D. Emfietzoglou / *Radiation Research 164 (2005) 202–211]*

Liquid water GOS

GOS properties

I-value = 77.955 eV



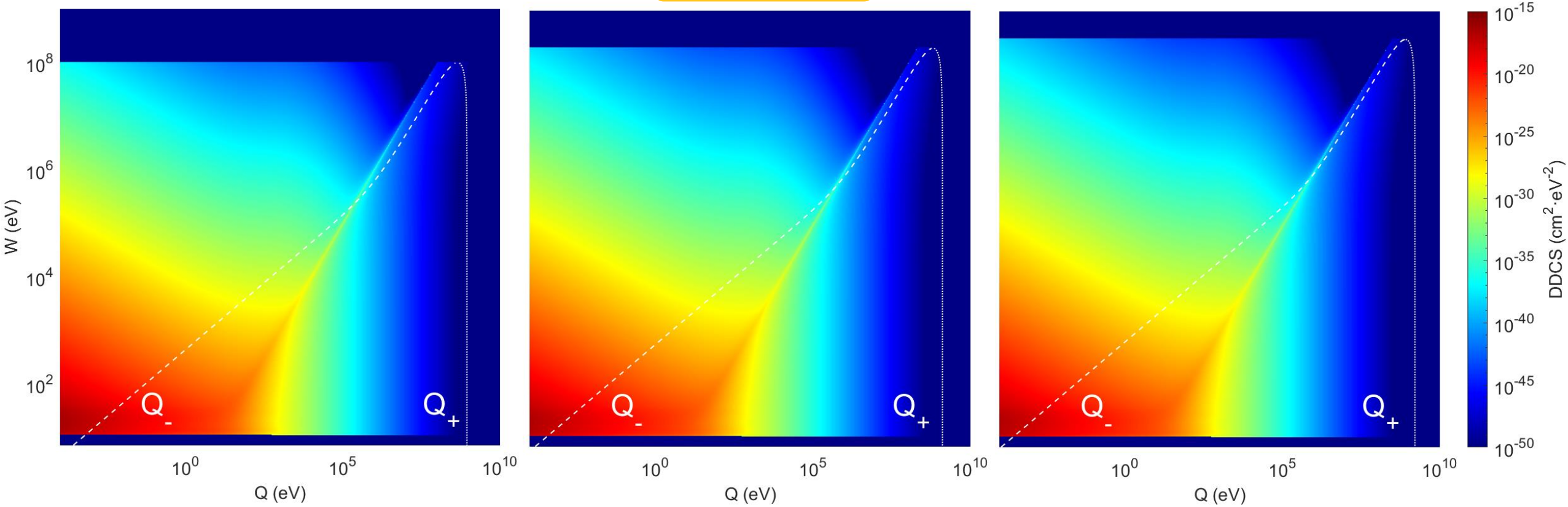
Datasets calculation

Ionisation DCS

$$\frac{d^2\sigma(Q,W)}{dW\,dQ} \longrightarrow \frac{d\sigma}{dW} = \int_{Q_-(W)}^{Q_+(W)} dQ \frac{d^2\sigma}{dW\,dQ}$$

$Q_\pm(E,W)$ Endpoints of the kinematically allowed recoil energy interval

$1b_1$ - shell



E = 100 MeV E = 200 MeV E = 300 MeV

Datasets calculation

Ionisation DCS

$$\frac{d^2\sigma(Q,W)}{dW\,dQ} \longrightarrow \frac{d\sigma}{dW} = \int_{Q_-(W)}^{Q_+(W)} dQ \frac{d^2\sigma}{dW\,dQ}$$

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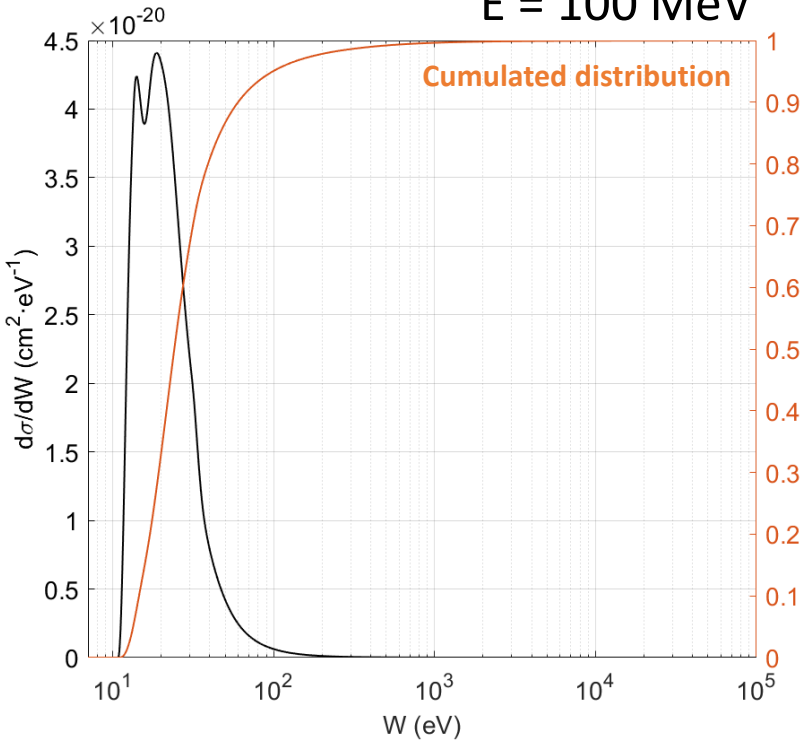
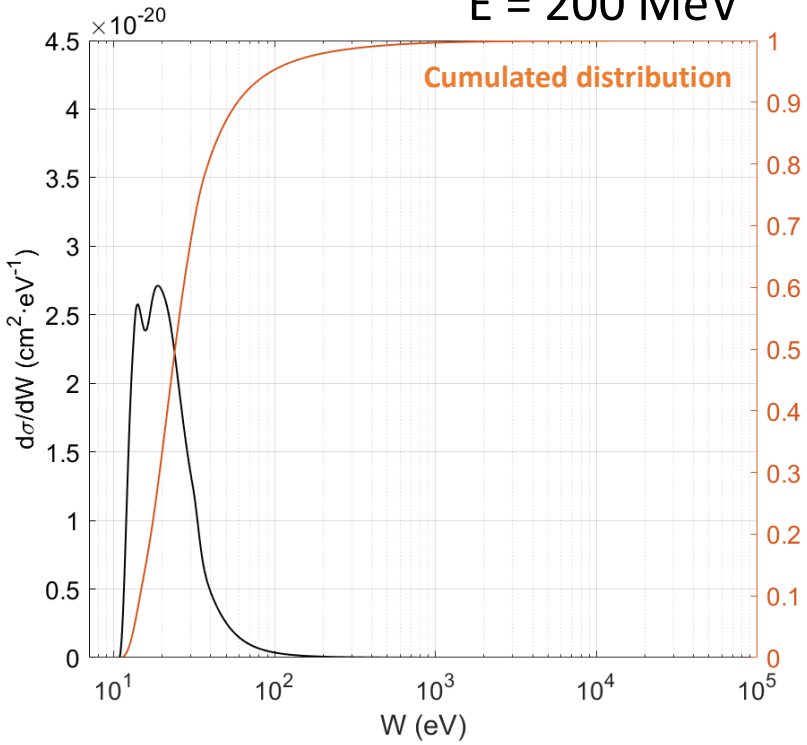
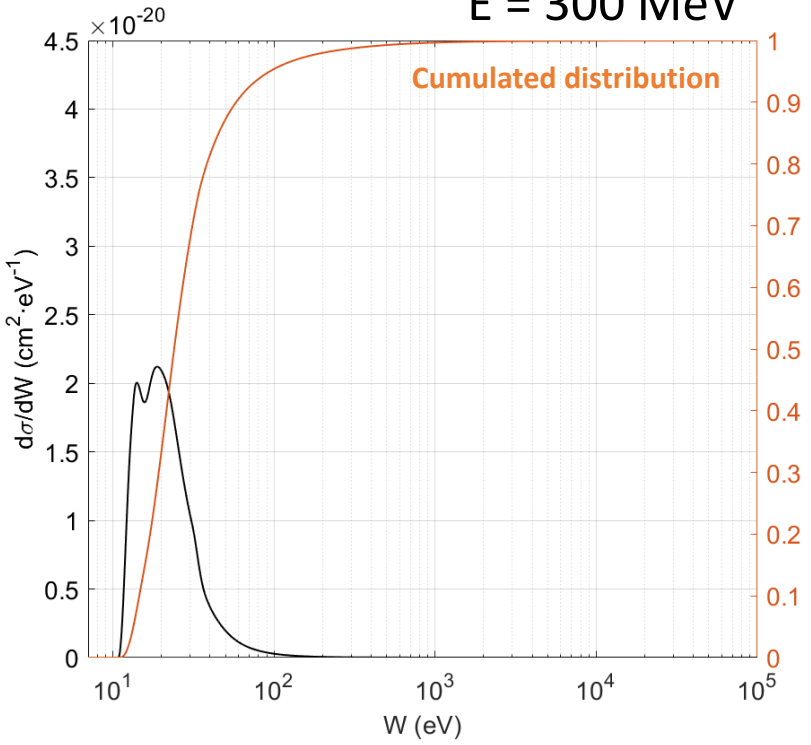


E = 200 MeV



E = 300 MeV

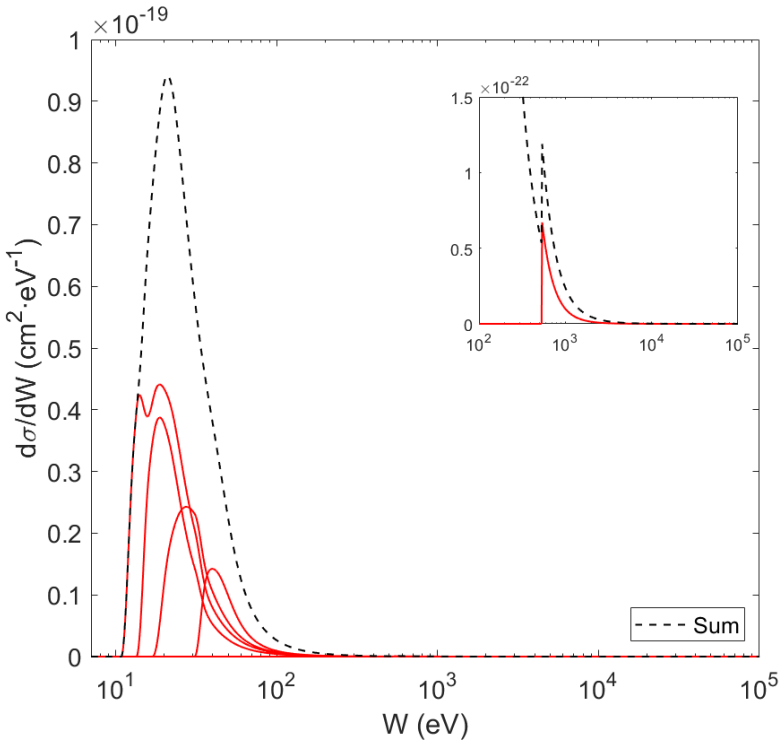


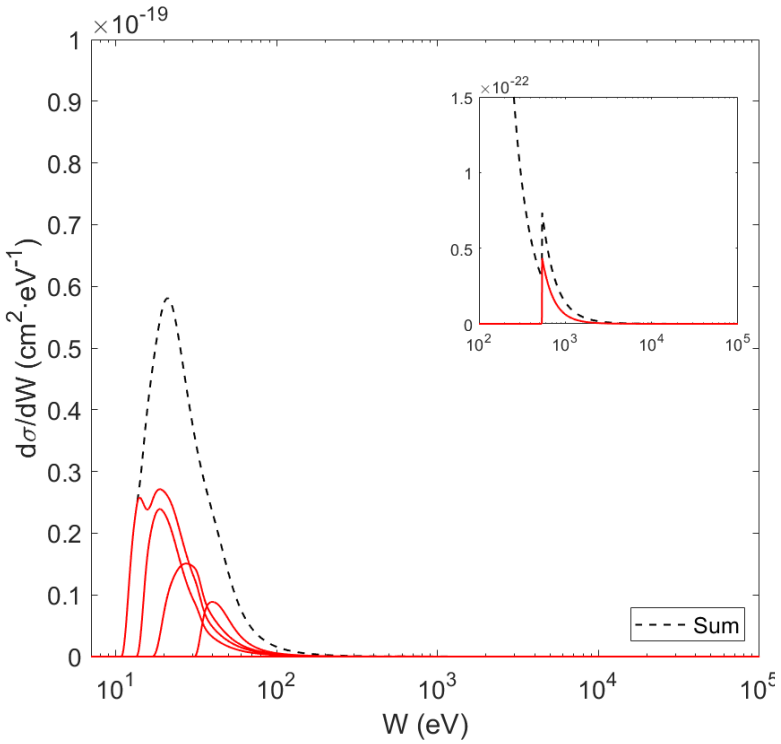
Datasets calculation

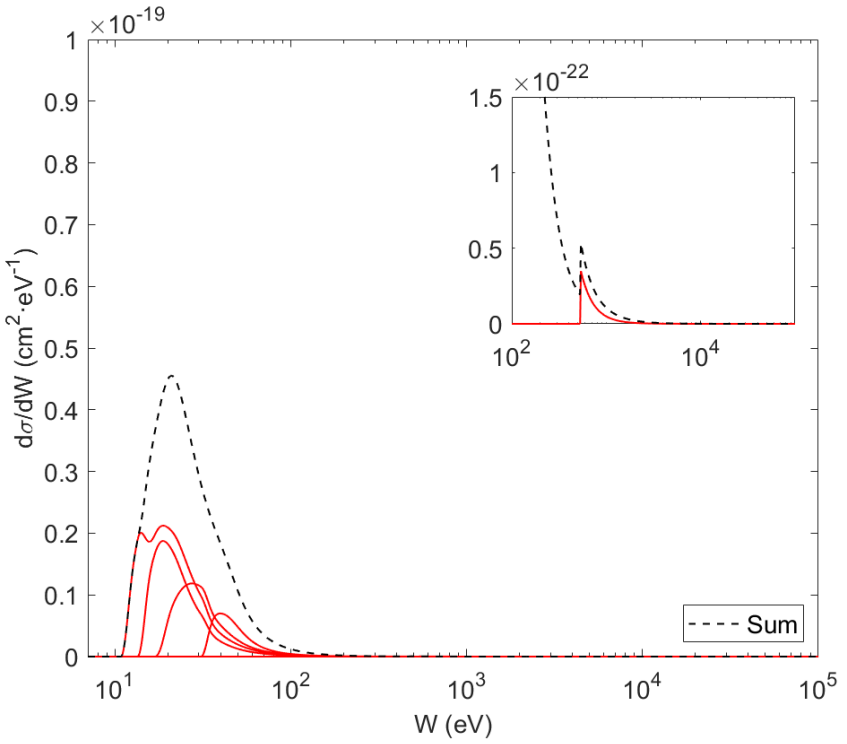
Ionisation DCS

$$\frac{d^2\sigma(Q,W)}{dW\,dQ} \longrightarrow \frac{d\sigma}{dW} = \int_{Q_-(W)}^{Q_+(W)} dQ \frac{d^2\sigma}{dW\,dQ}$$

$Q_\pm(E,W)$ Endpoints of the kinematically allowed recoil energy interval







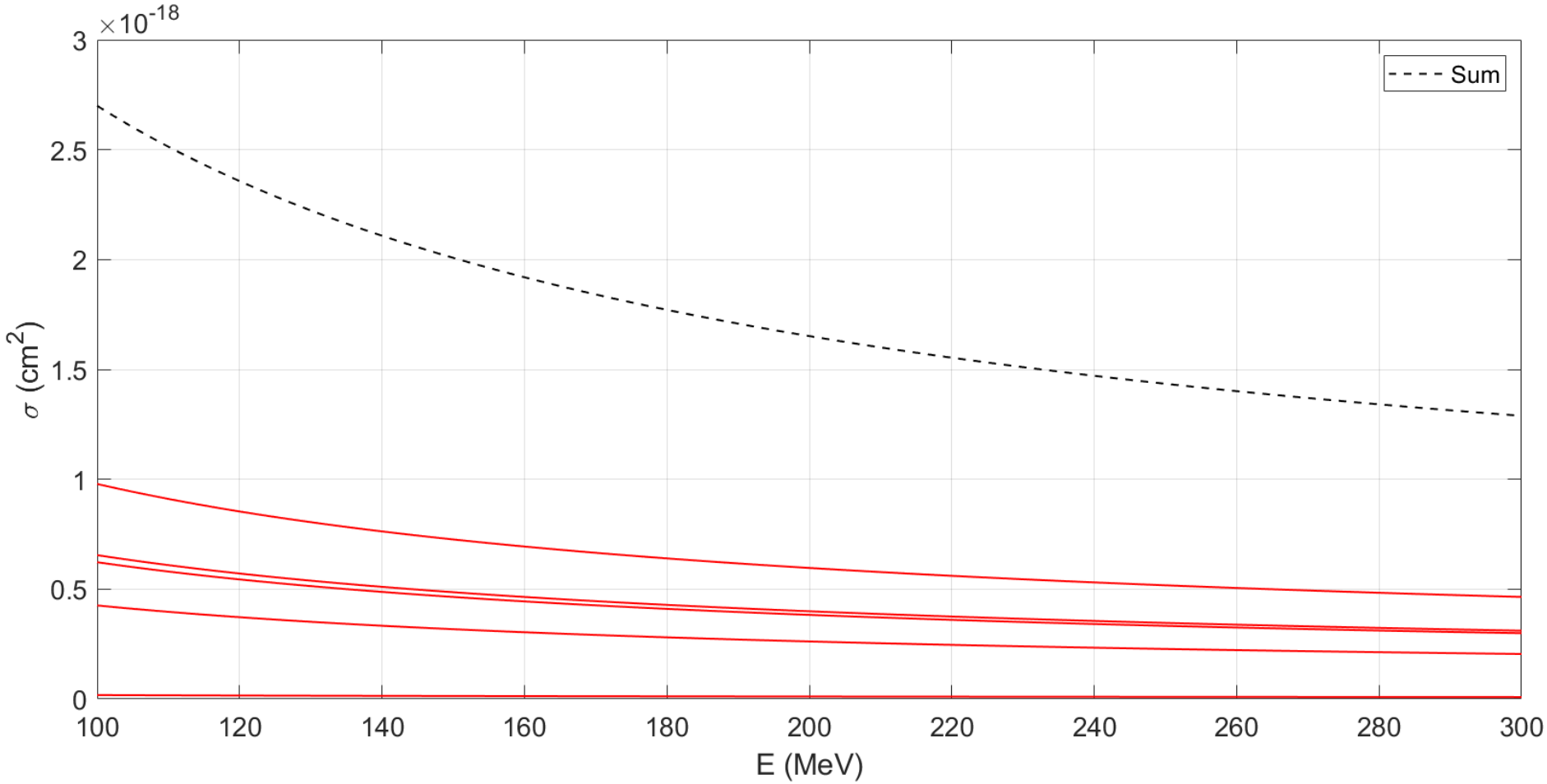
New data files!! sigmadiff_ionisation_p_RPWBA sigmadiff_cumulated_ionisation_p_RPWBA

Datasets calculation

Ionisation CS

$$\frac{d\sigma}{dW} \longrightarrow \sigma = \int_0^E dW \frac{d\sigma}{dW}$$

New data file!! sigma_ionisation_p_RPWBA



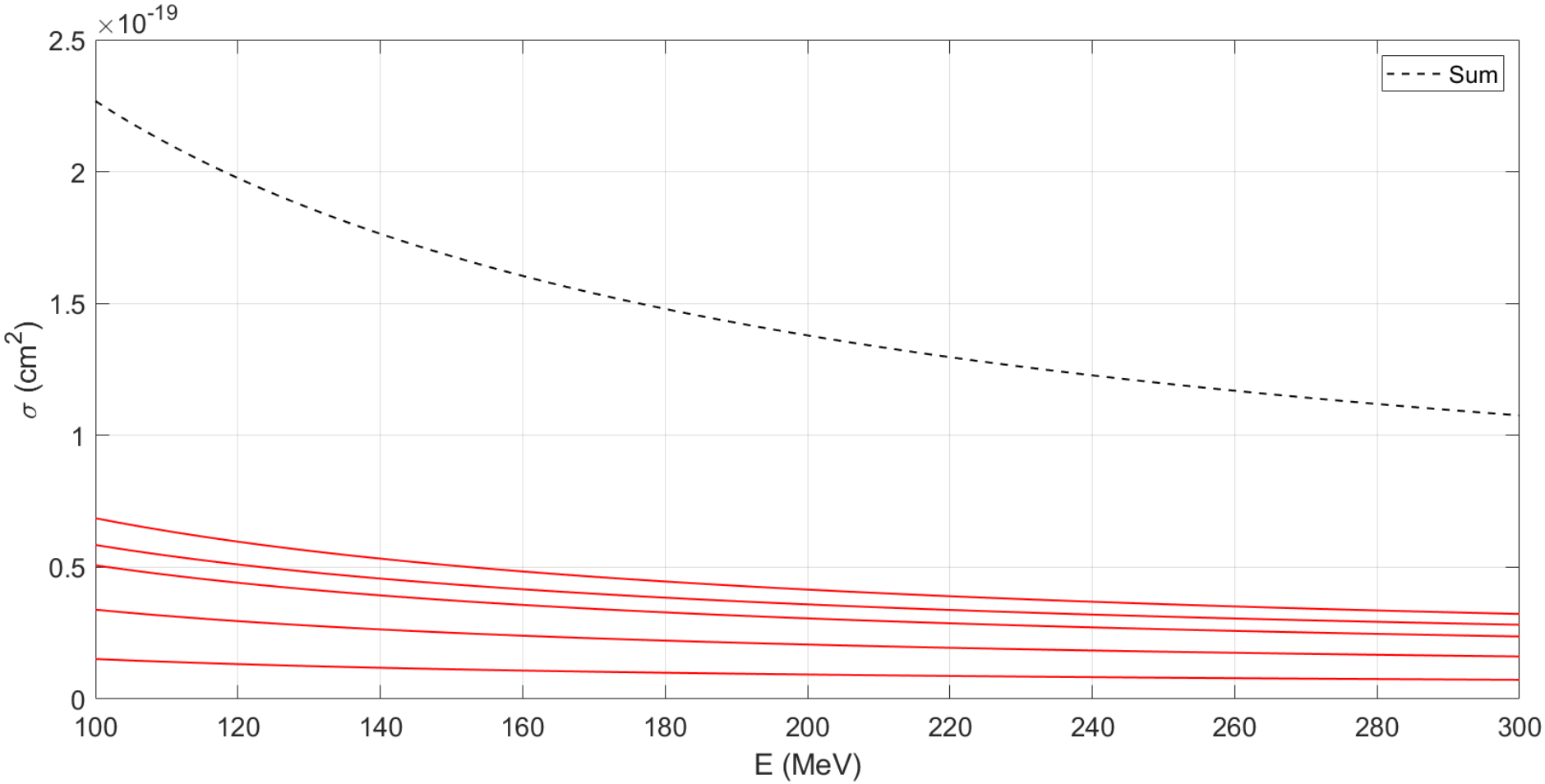
Datasets calculation

Excitation CS

$$\frac{df_{\mathrm{exc}}(Q,W)}{dW} = f_{\mathrm{exc}}(Q)\delta(W - W_{\mathrm{exc}}) \rightarrow \frac{d^2\sigma(Q,W)}{dW\,dQ} \rightarrow \sigma = \int_0^E dW \int_{Q_-(W)}^{Q_+(W)} dQ \frac{d^2\sigma}{dW\,dQ}$$

New data file!!

sigma_excitation_p_RPWBA



Implementation

G4DNARPWBAIonisationModel.cc

Models

G4DNARPWBAExcitationModel.cc

Datasets

- sigma_ionisation_p_RPWBA
- sigma_excitation_p_RPWBA

Processes

G4DNAIonisation.cc

```
else if(name == "proton")
{
  if(!EmModel(0)) // MK: Is this a correct test ?
  {
    G4DNAMillerGreenExcitationModel* miller =
        new G4DNAMillerGreenExcitationModel();
    SetEmModel(miller);
    miller->SetLowEnergyLimit(10 * eV);
    miller->SetHighEnergyLimit(500 * keV);

    G4DNABornExcitationModel* born = new G4DNABornExcitationModel();
    SetEmModel(born);
    born->SetLowEnergyLimit(500 * keV);
    born->SetHighEnergyLimit(100 * MeV);

    G4DNARPWBAExcitationModel* RPWBA = new G4DNARPWBAExcitationModel();
    SetEmModel(RPWBA);
    RPWBA->SetLowEnergyLimit(100 * MeV);
    RPWBA->SetHighEnergyLimit(300 * MeV);
  }
```

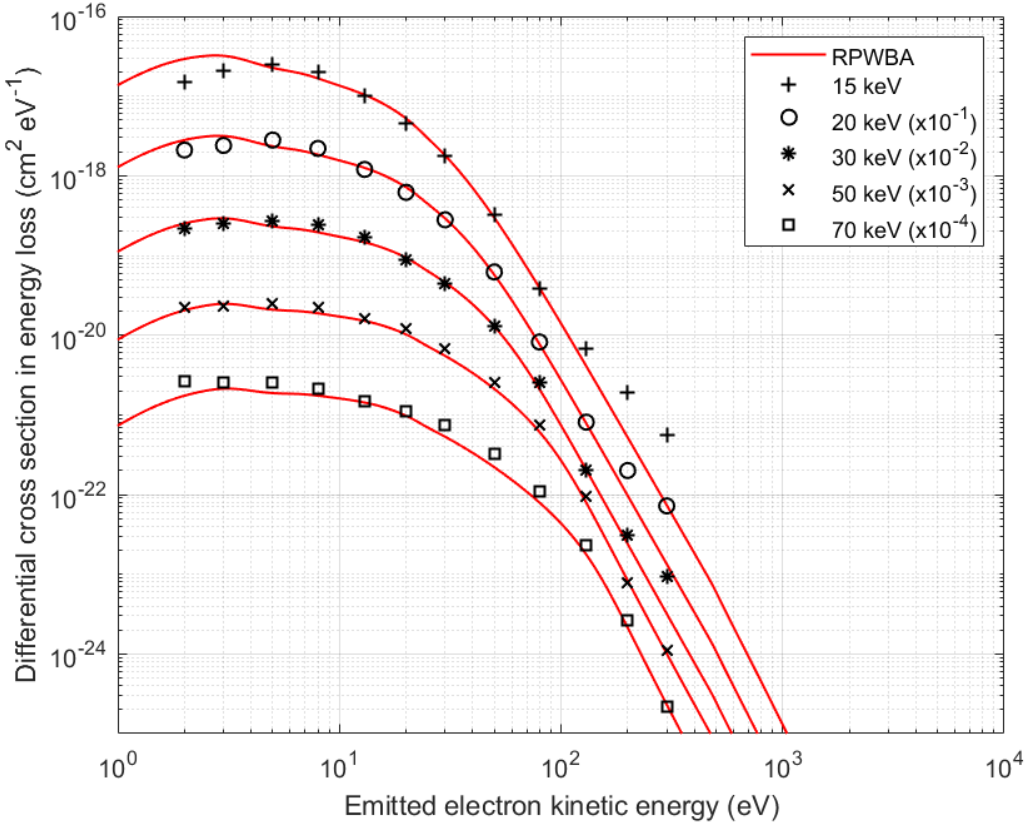
G4DNAExcitation.cc

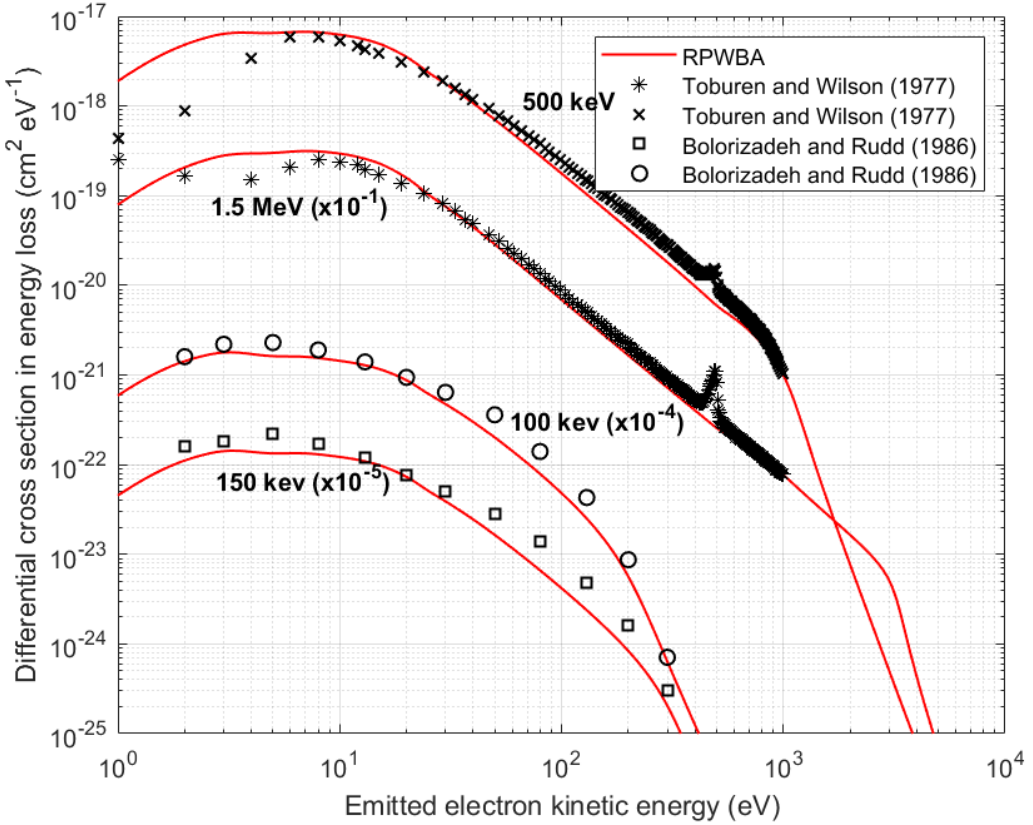
```
else if(name == "proton")
{
  if(!EmModel(0)) // MK: Is this a correct test ?
  {
    G4DNAMillerGreenExcitationModel* miller =
        new G4DNAMillerGreenExcitationModel();
    SetEmModel(miller);
    miller->SetLowEnergyLimit(10 * eV);
    miller->SetHighEnergyLimit(500 * keV);

    G4DNABornExcitationModel* born = new G4DNABornExcitationModel();
    SetEmModel(born);
    born->SetLowEnergyLimit(500 * keV);
    born->SetHighEnergyLimit(100 * MeV);

    G4DNARPWBAExcitationModel* RPWBA = new G4DNARPWBAExcitationModel();
    SetEmModel(RPWBA);
    RPWBA->SetLowEnergyLimit(100 * MeV);
    RPWBA->SetHighEnergyLimit(300 * MeV);
  }
```

Validation

Ionisation DCS

Experimental data for **vapour water**

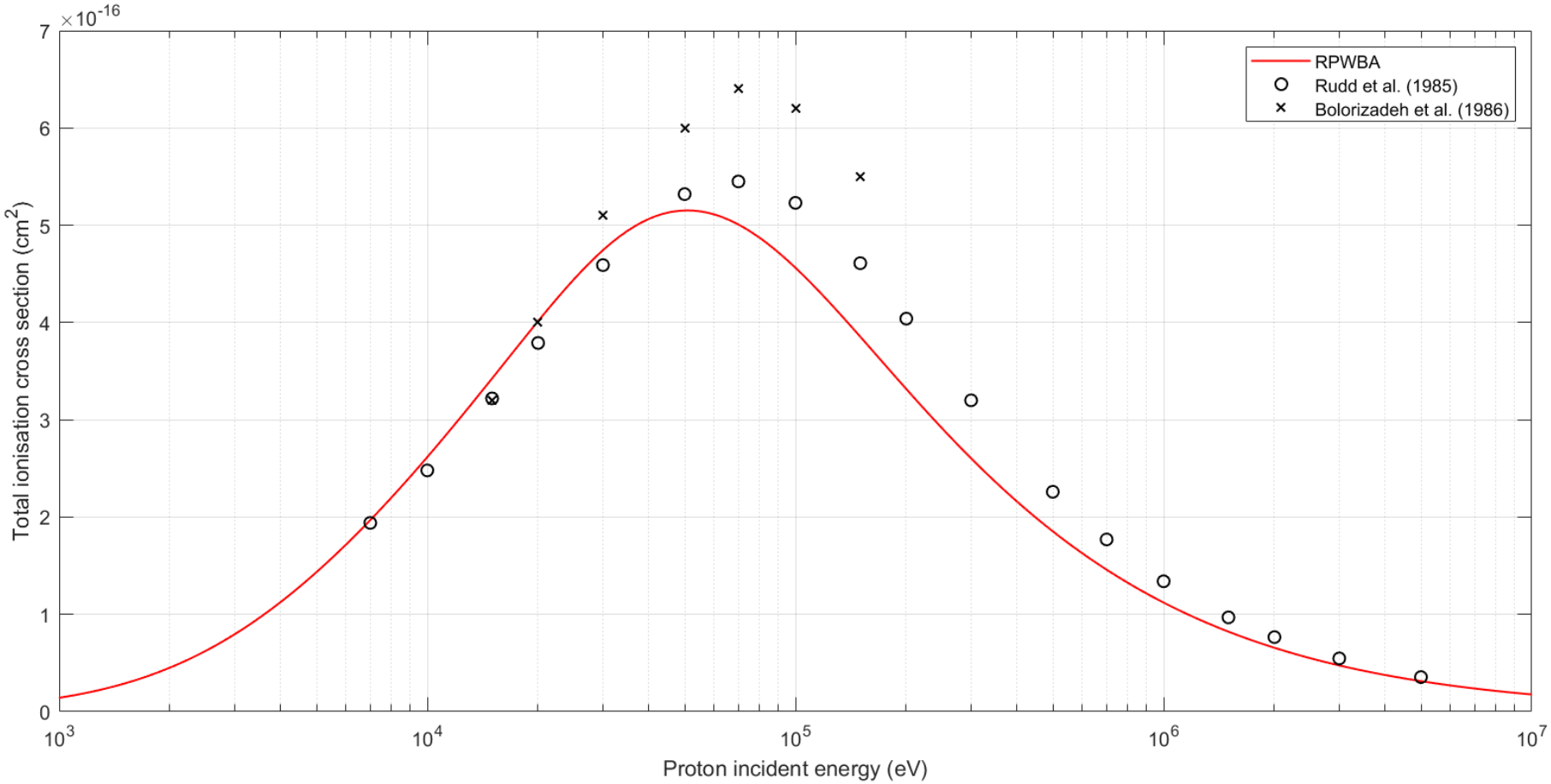




Validation

Ionisation CS

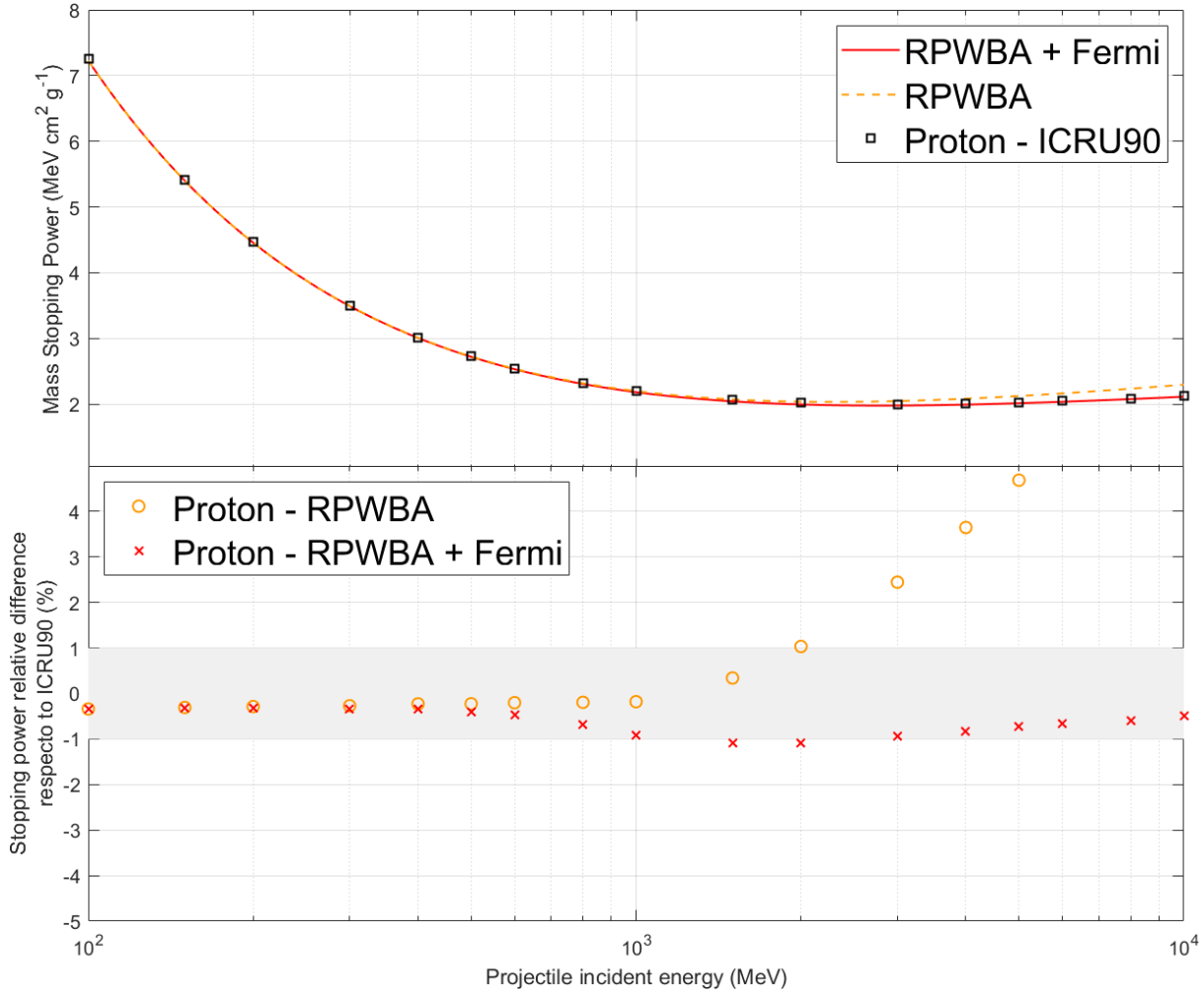
Experimental data for **vapour water**



Validation

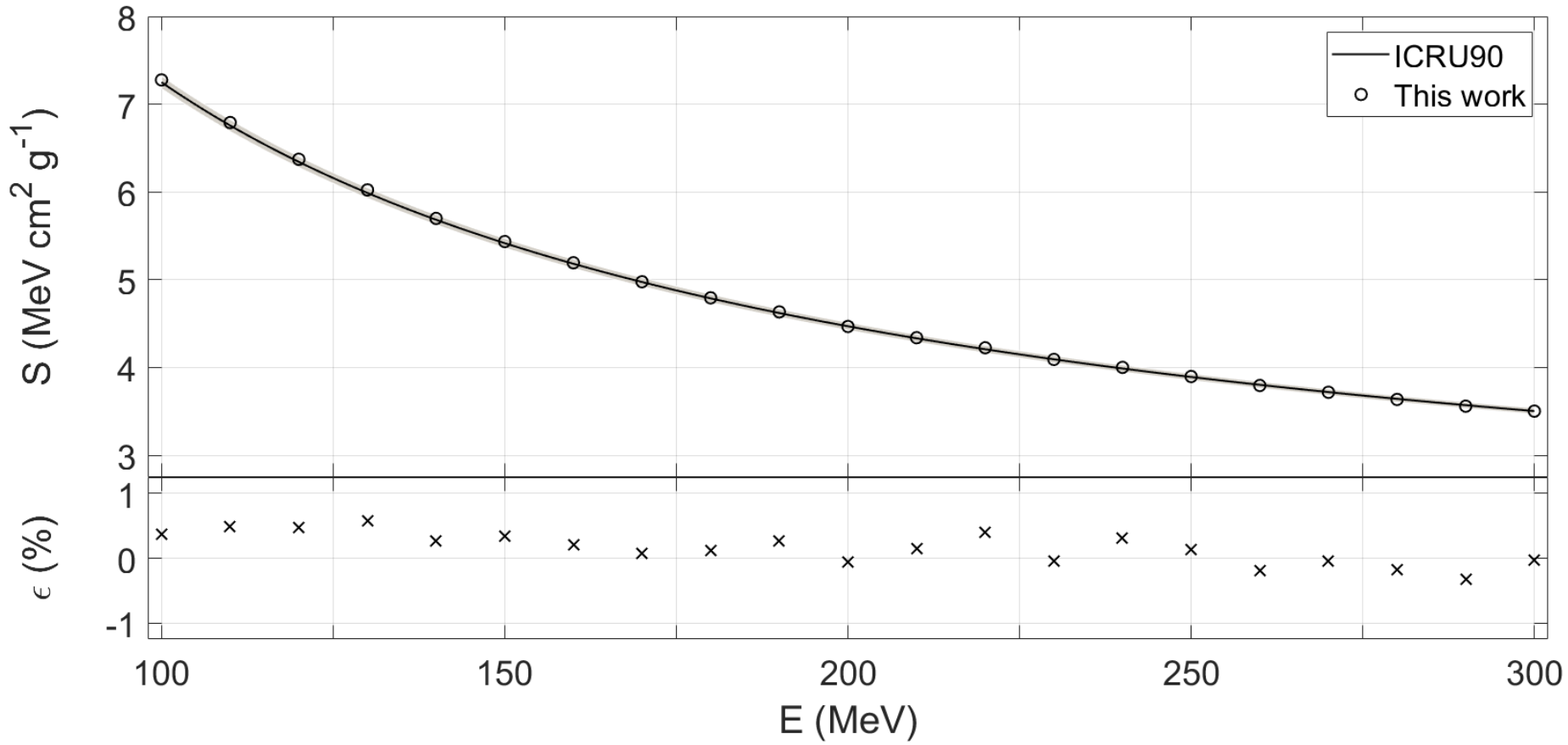
Stopping power

Fermi density effect



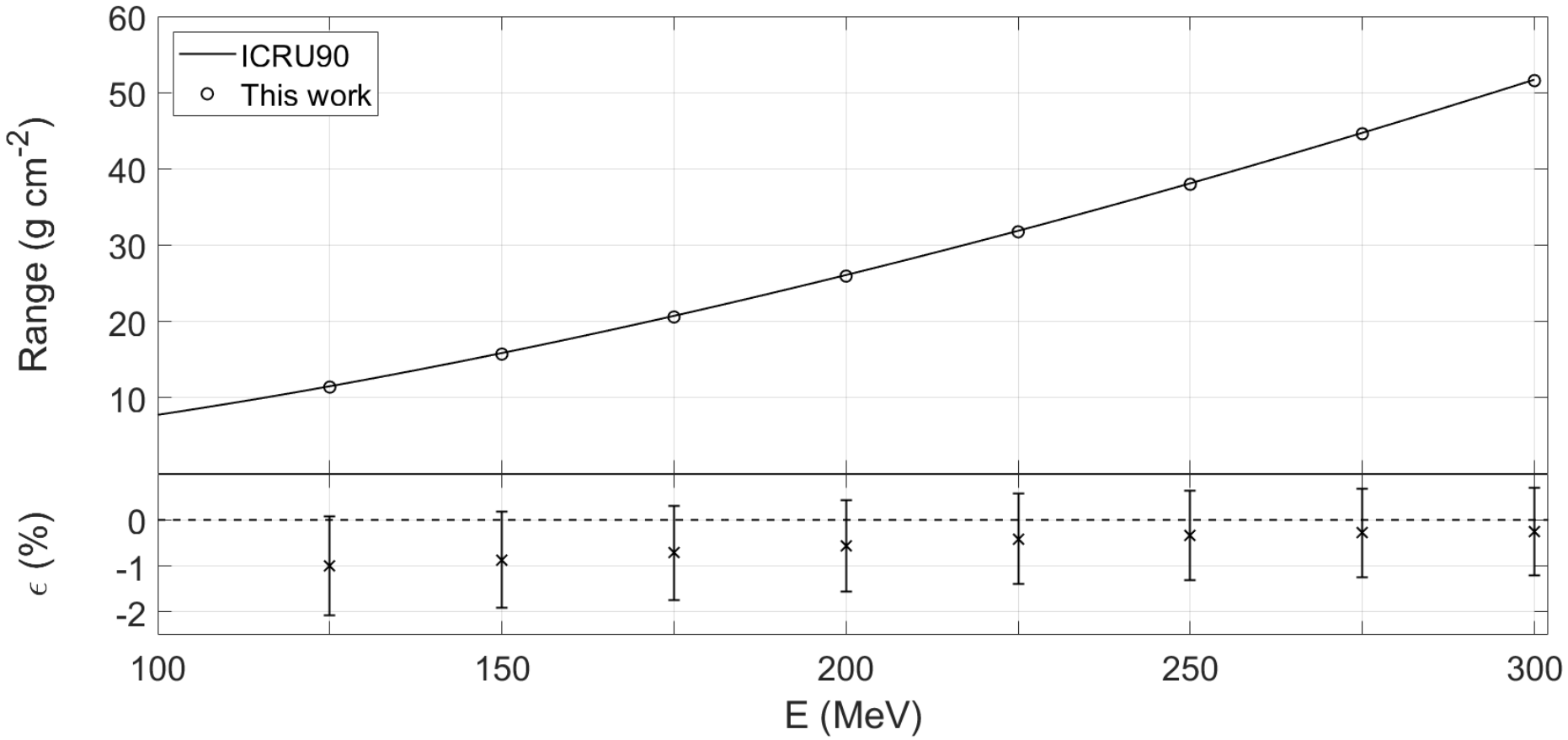
Implementation verification

spower example



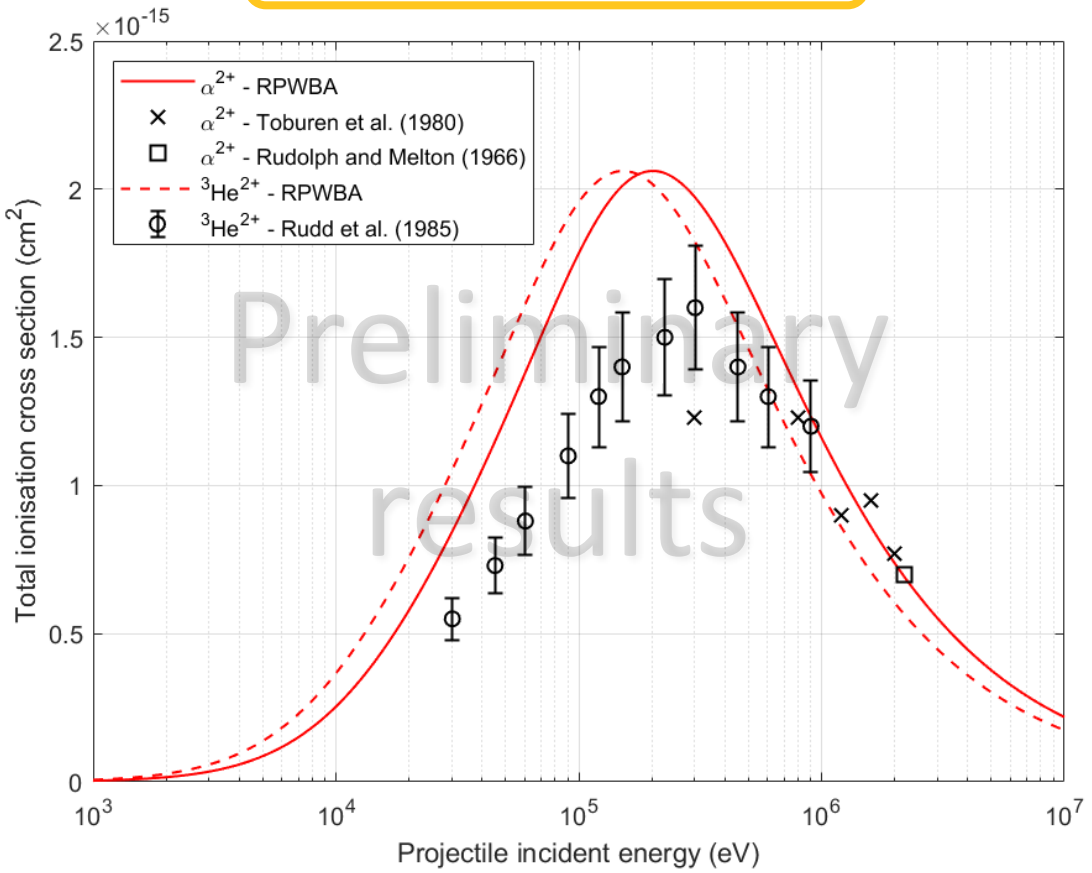
Implementation verification

range example



Future perspectives

Alpha interaction



Hydrogen interaction