The new “RPWBA” model implemented in Geant4-DNA for proton ionization and excitation of liquid water above 100 MeV

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Motivation and goal

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

PROTONS (named "proton")

Liquid water

- **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

Max. energy Limit → **100 MeV**

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

Range in liquid water → ≈ 39 cm

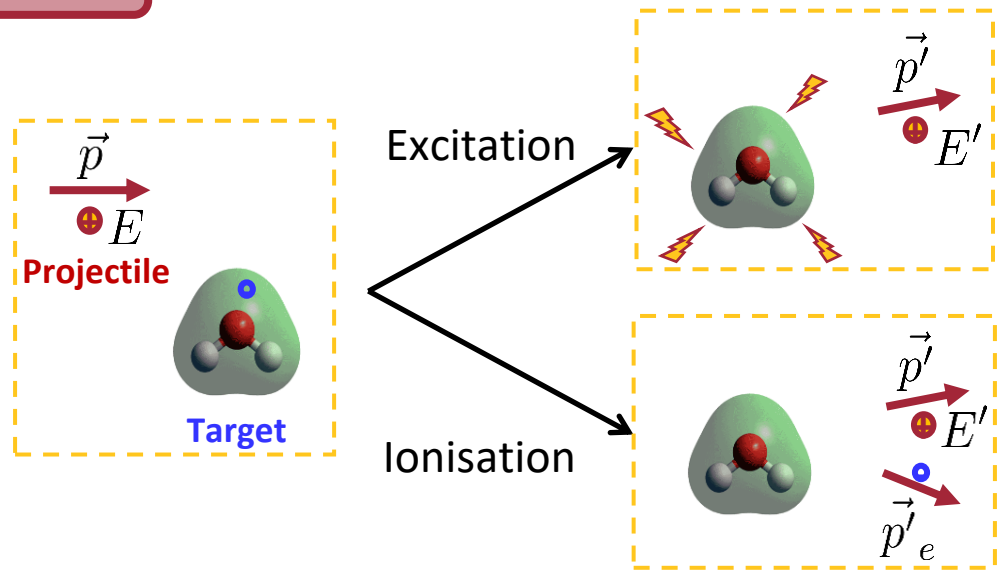
- **Ionisation** G4DNAIonisation
  - G4DNARuddIonisationModel (G4DNARuddIonisationExtendedModel is also usable, °)
    - applicable energy range : 0 eV - 500 keV
    - cut at 100 eV (5)
    - type : interpolated
    - constructors : default, option2 (°), option4, option6
  - G4DNABornIonisationModel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

Increase these limits!

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

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

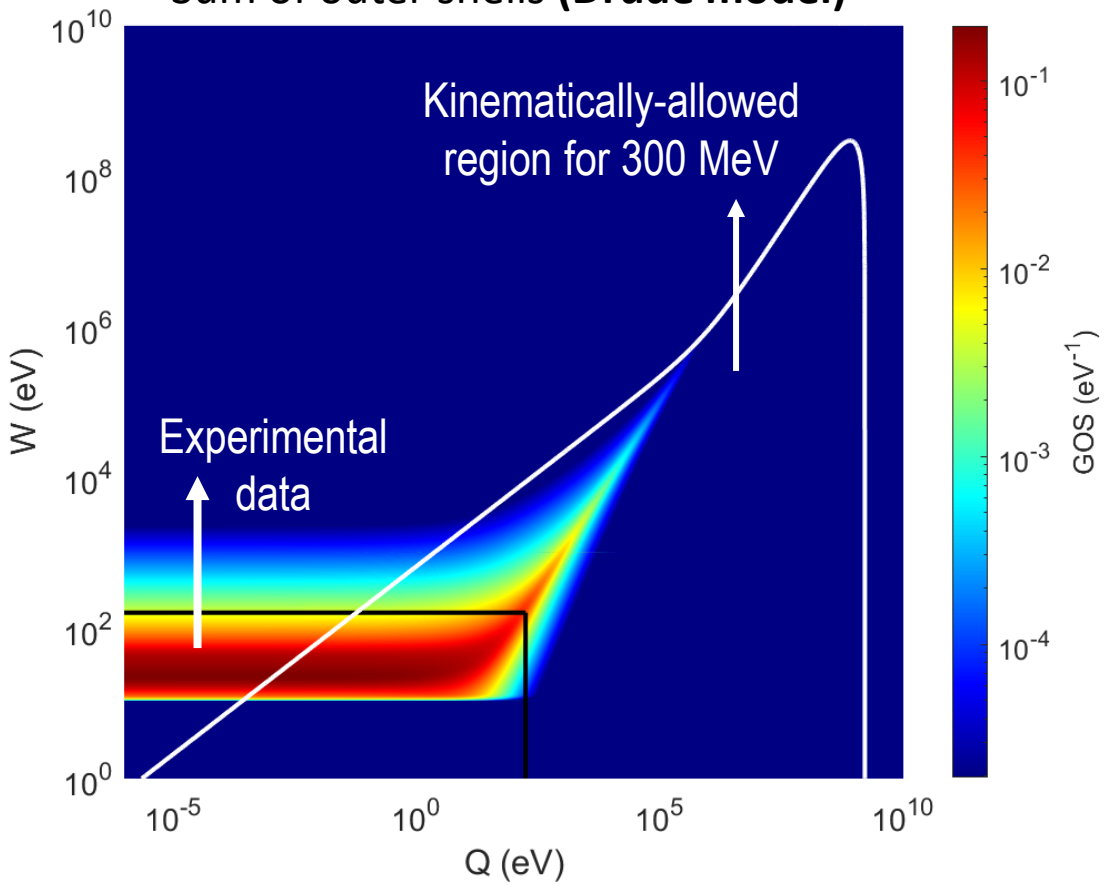
Generalized oscillator strength (GOS)

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

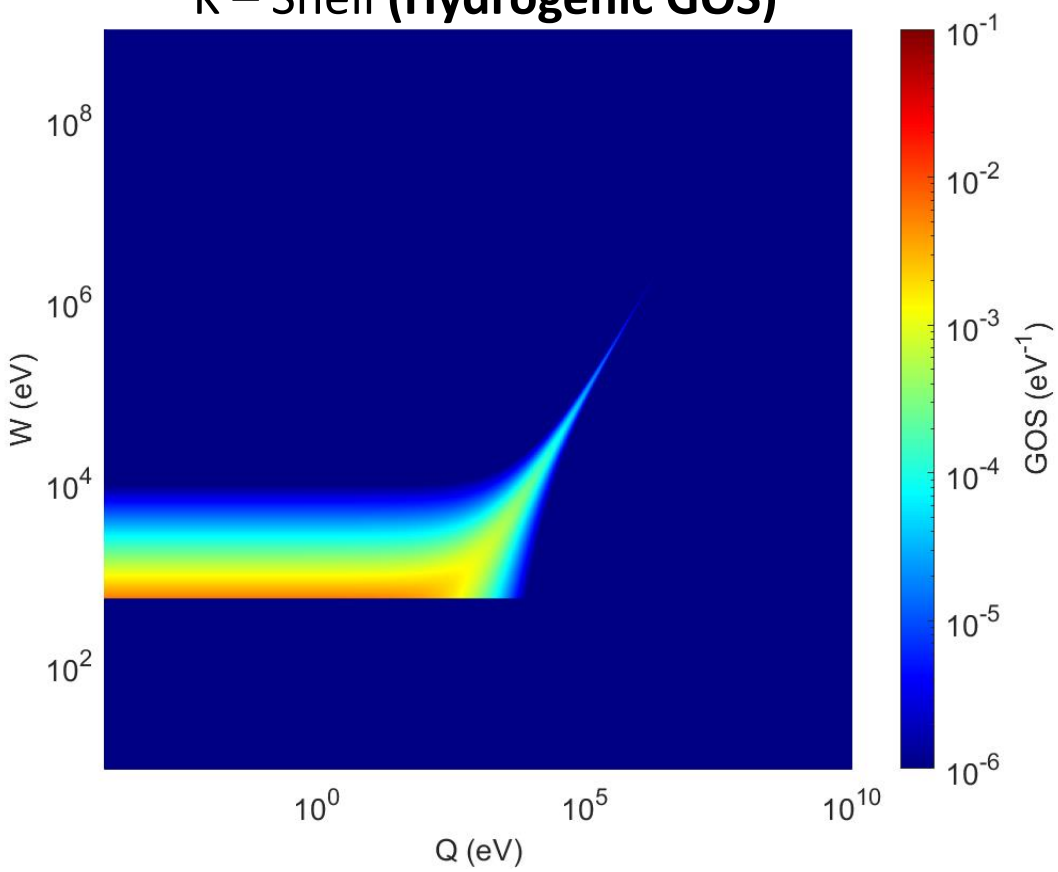
Liquid Water GOS

Ionisation GOS

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



K – Shell **(Hydrogenic GOS)**

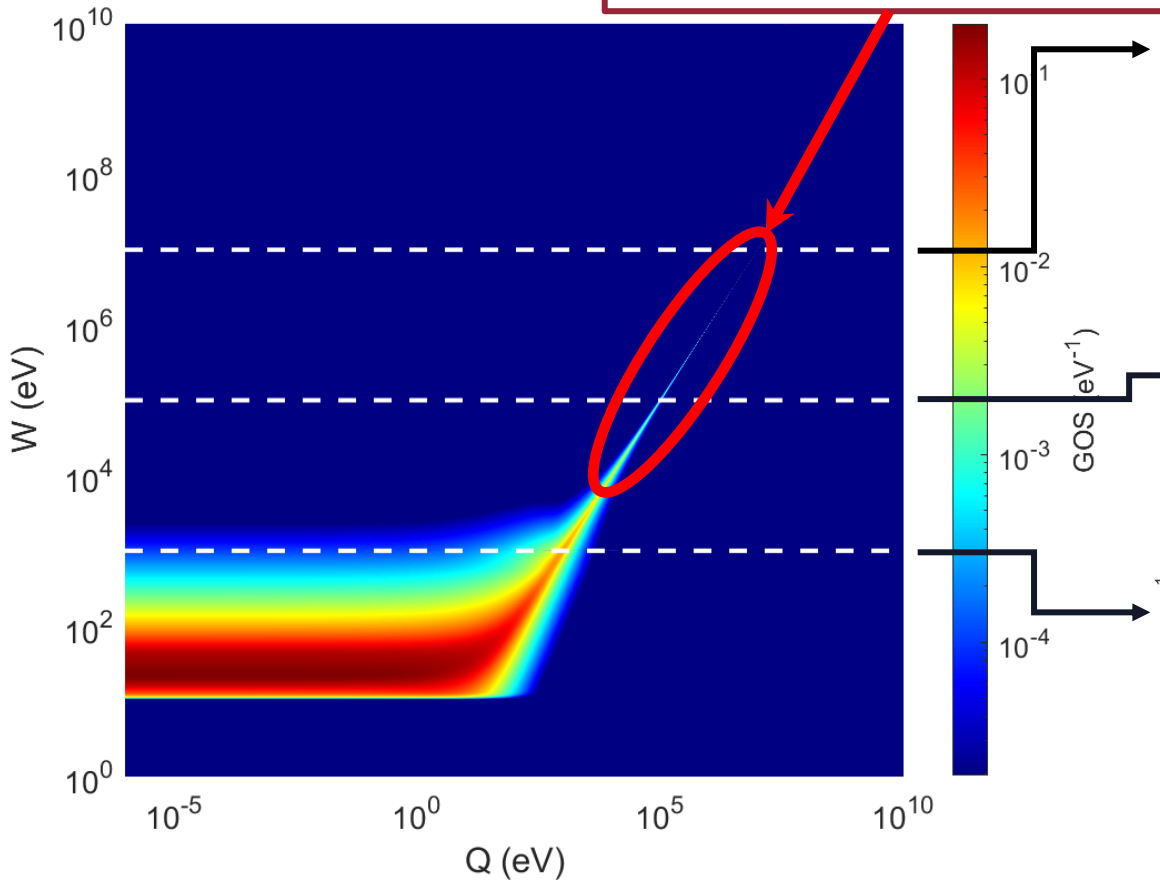


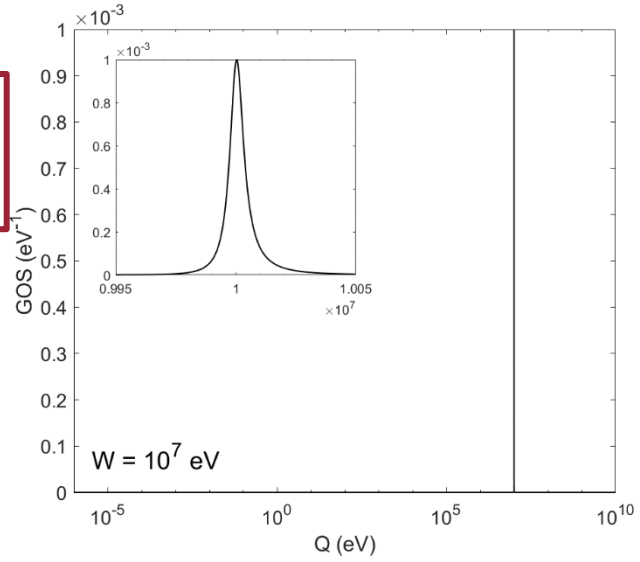
Parameters values taken from [D. Emfietzoglou / *Radiation Research 164 (2005) 202–211]*

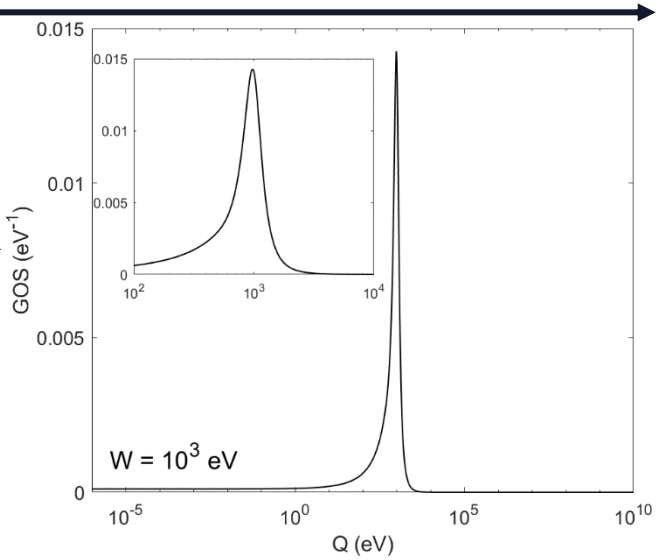
Liquid Water GOS

Ionisation GOS

Sum of outer shells **(Drude model)**
+
Born-Compton profile extension

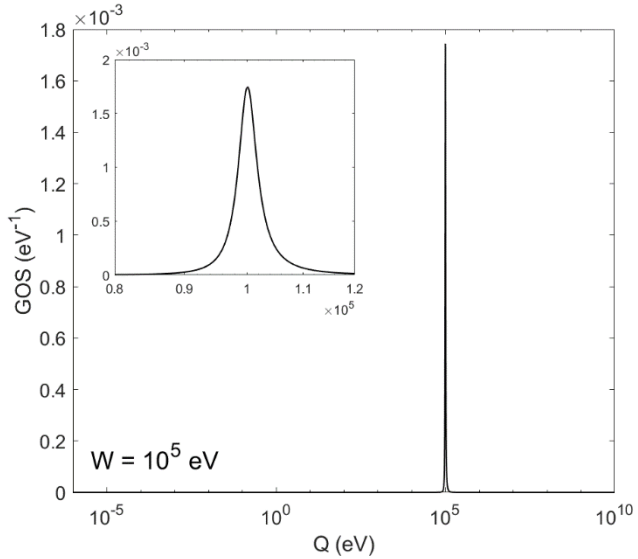






Adaptative grid to reproduce numerically the Bethe-Ridge accurately

Necessary for numerical integration of DDCS

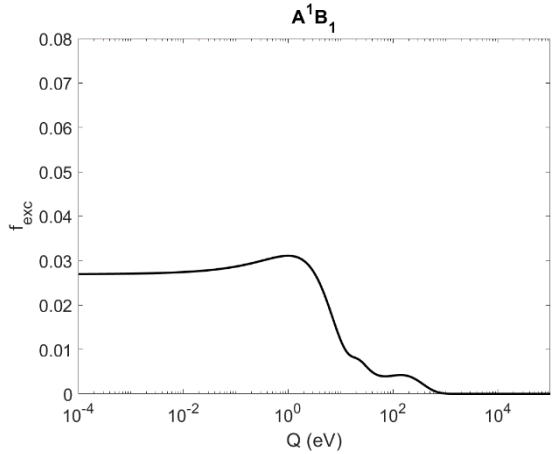


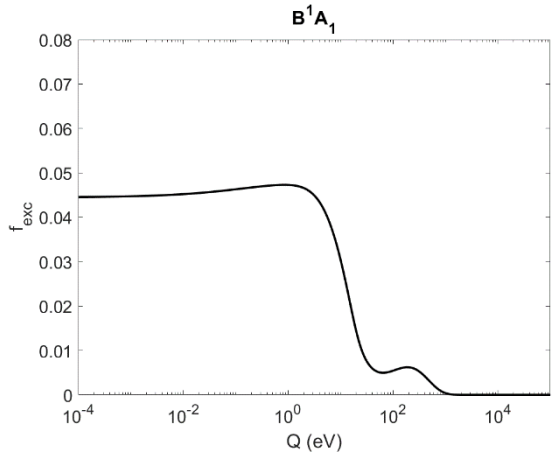
Liquid Water GOS

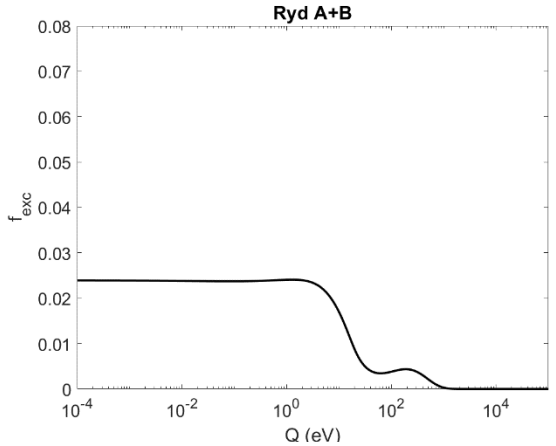
Excitation GOS

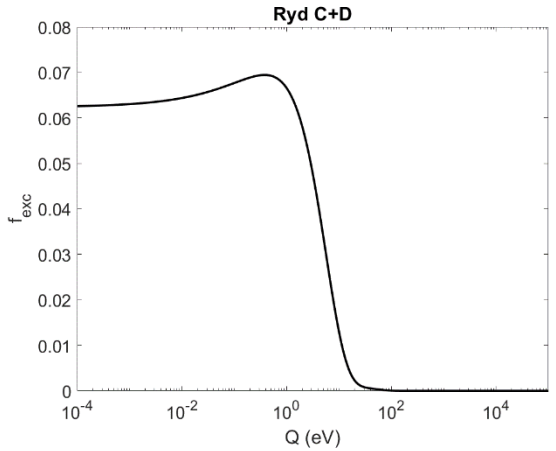
$$\frac{df_{\mathrm{exc}}(Q,W)}{dW} = f_{\mathrm{exc}}(Q)\delta(W - W_{\mathrm{exc}})$$

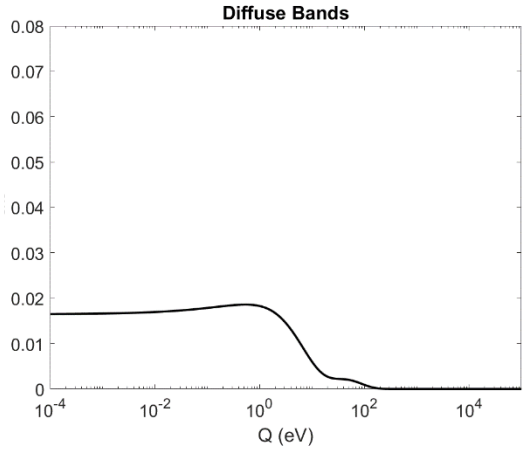
Discrete transitions











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

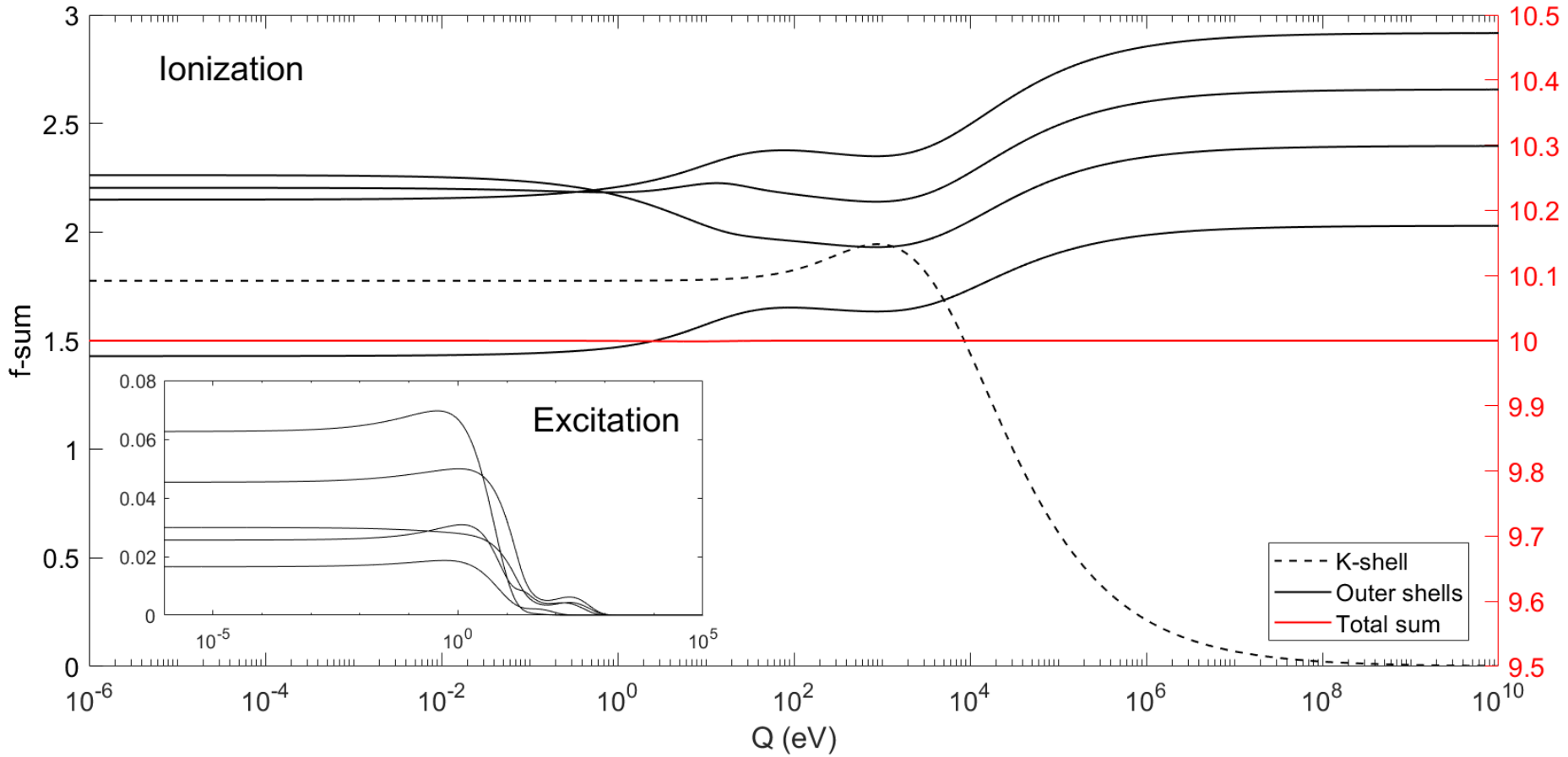
Parameters values taken from

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

Liquid Water GOS

GOS properties

***I*-value = 77.955 eV**



Calculation of datasets

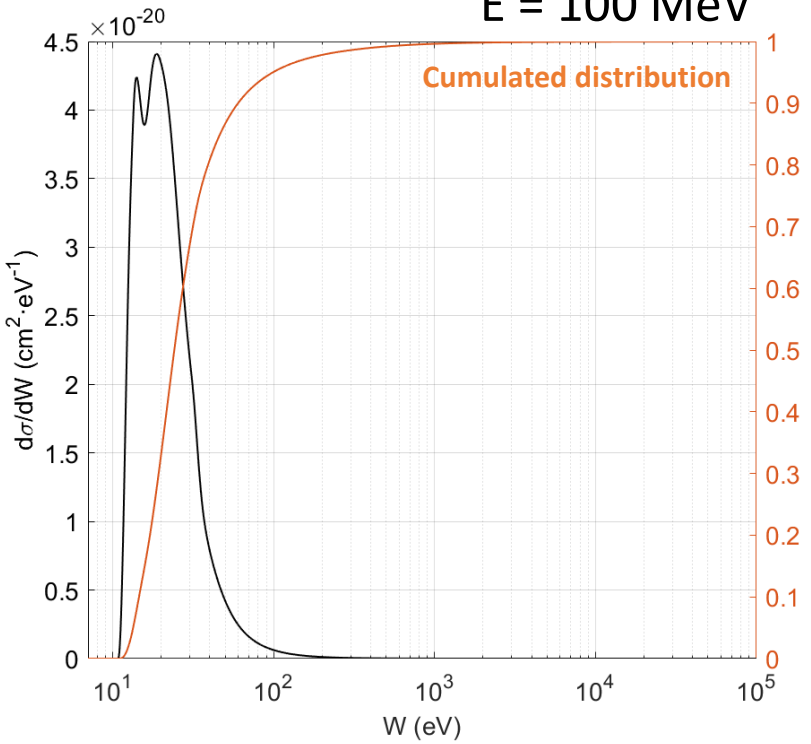
Ionisation DCS

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

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

$1b_1$ - shell

E = 100 MeV



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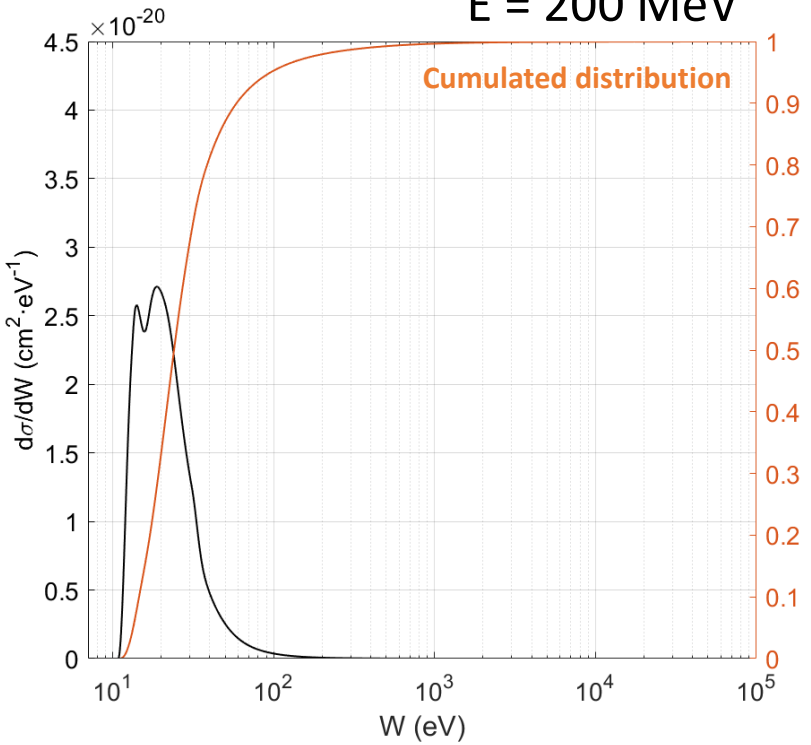
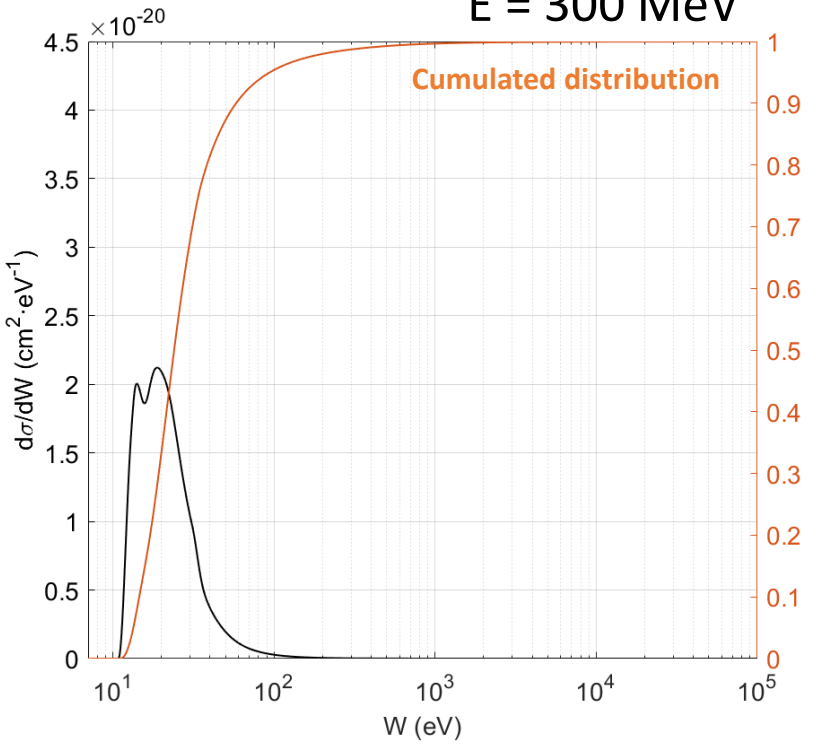


E = 300 MeV



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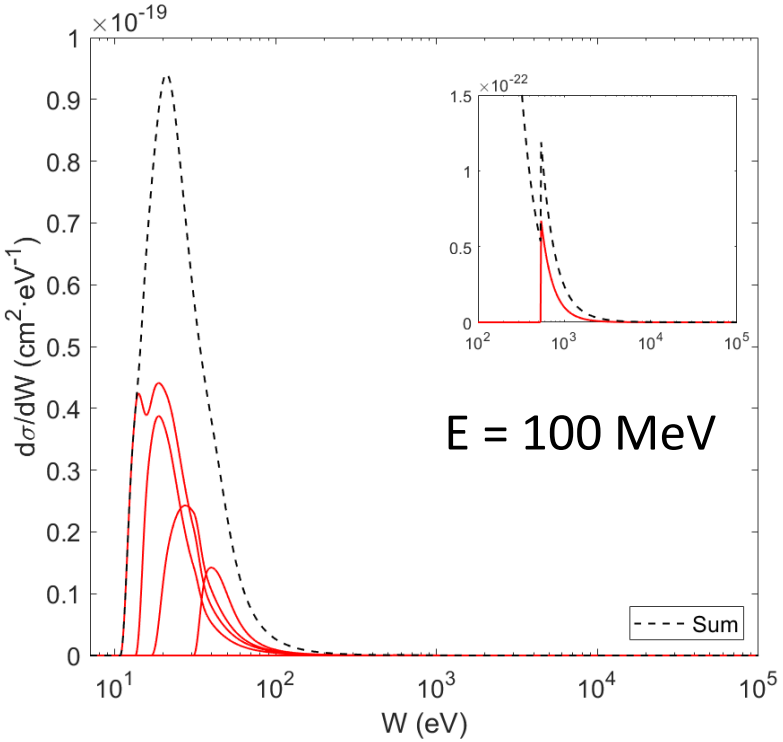
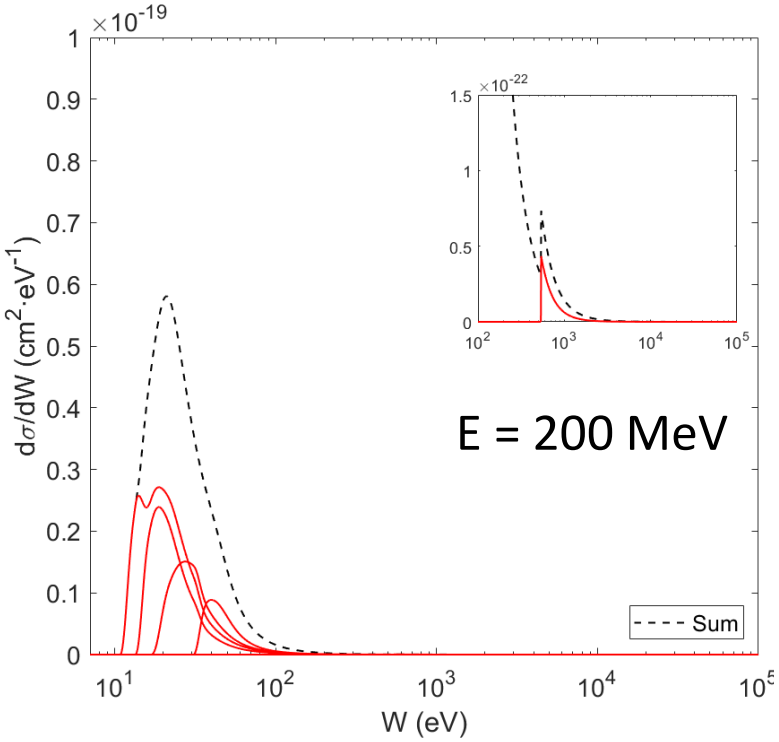
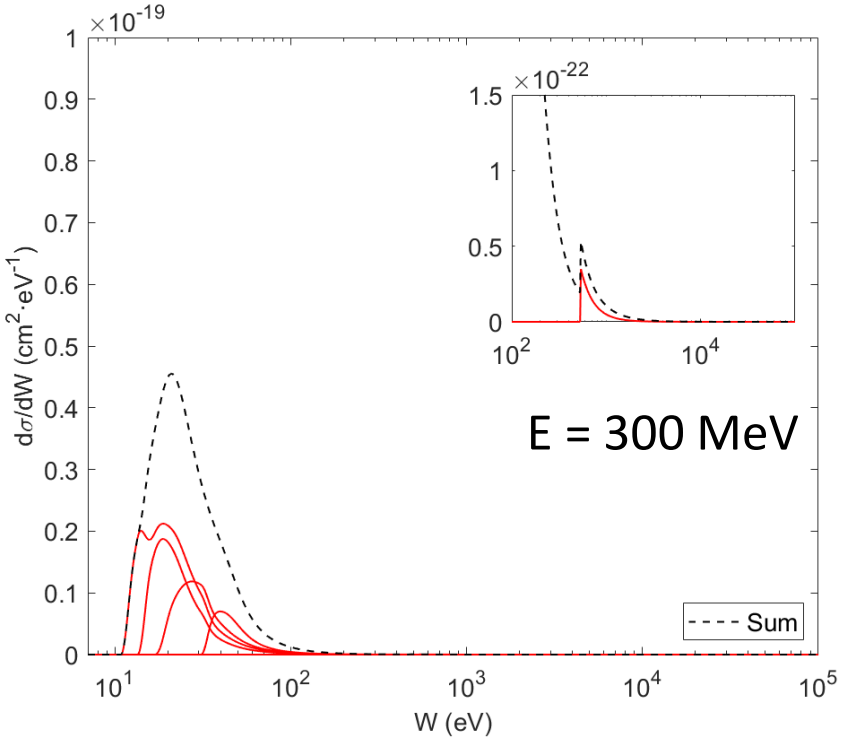
$Q_\pm(E,W)$ Endpoints of the kinematically allowed recoil energy interval







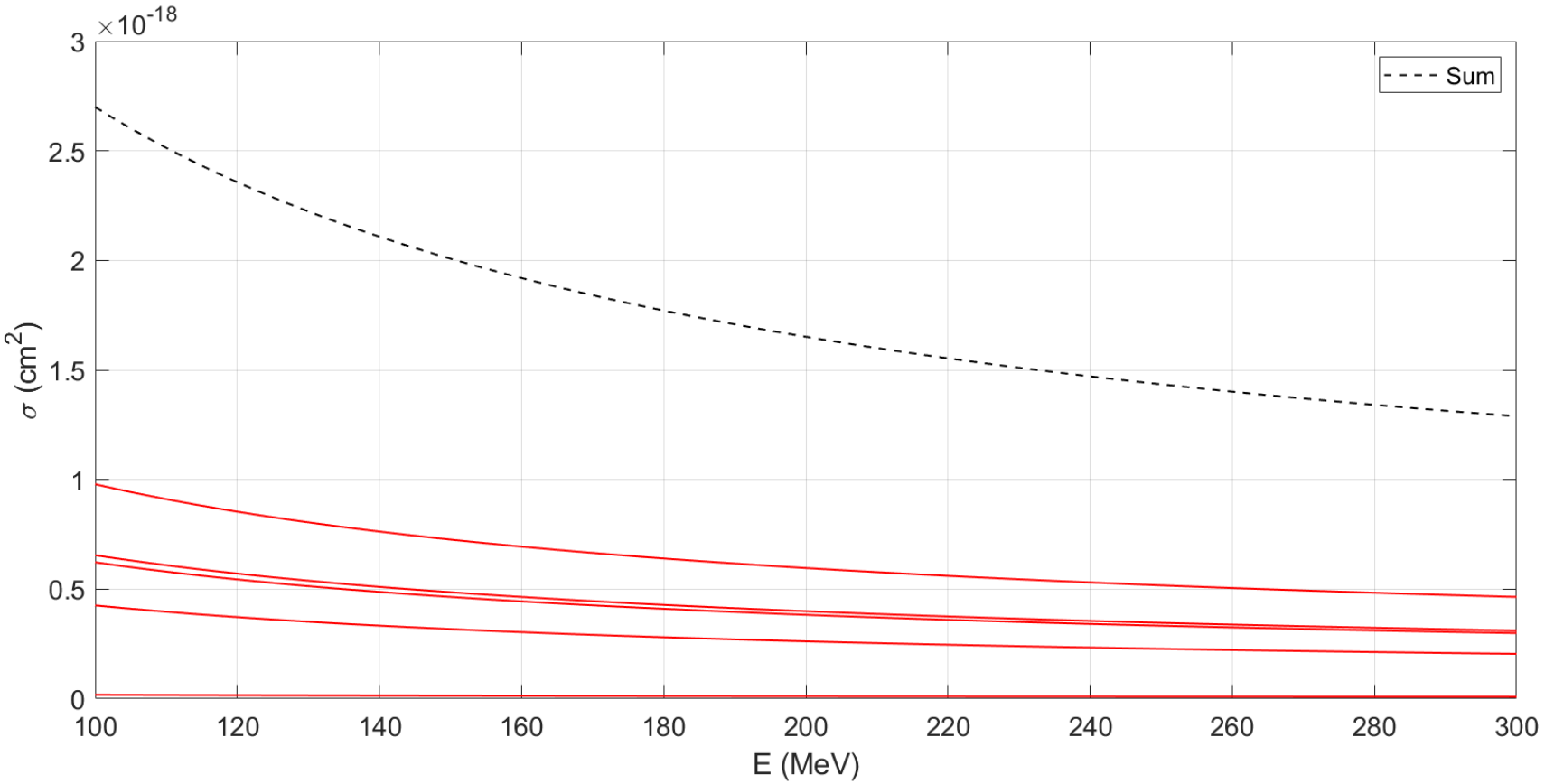
New data files from G4EMLOW8.1 →

- sigmadiff_ionisation_p_RPWBA
- sigmadiff_cumulated_ionisation_p_RPWBA

Calculation of datasets

Ionisation CS

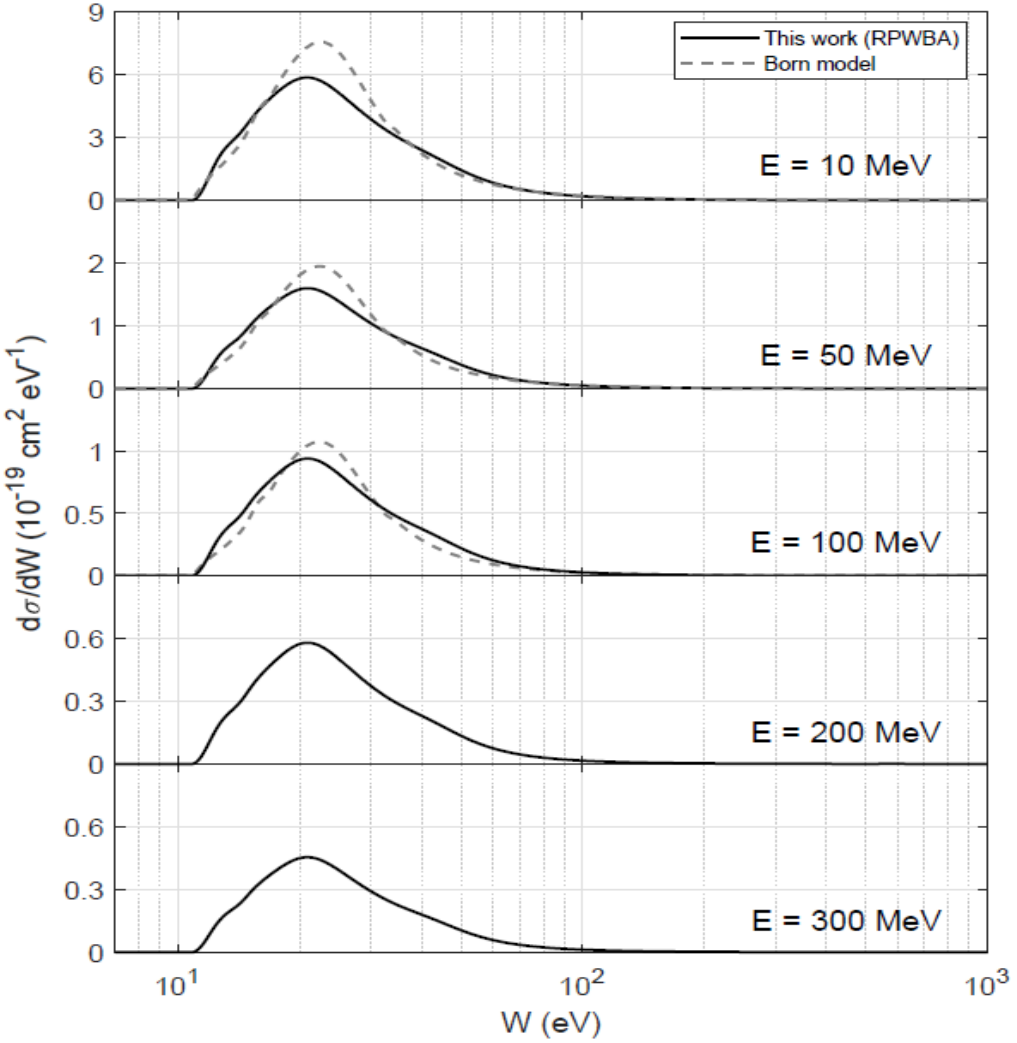
$$\frac{d\sigma}{dW} \longrightarrow \sigma = \int_0^E dW \frac{d\sigma}{dW}$$



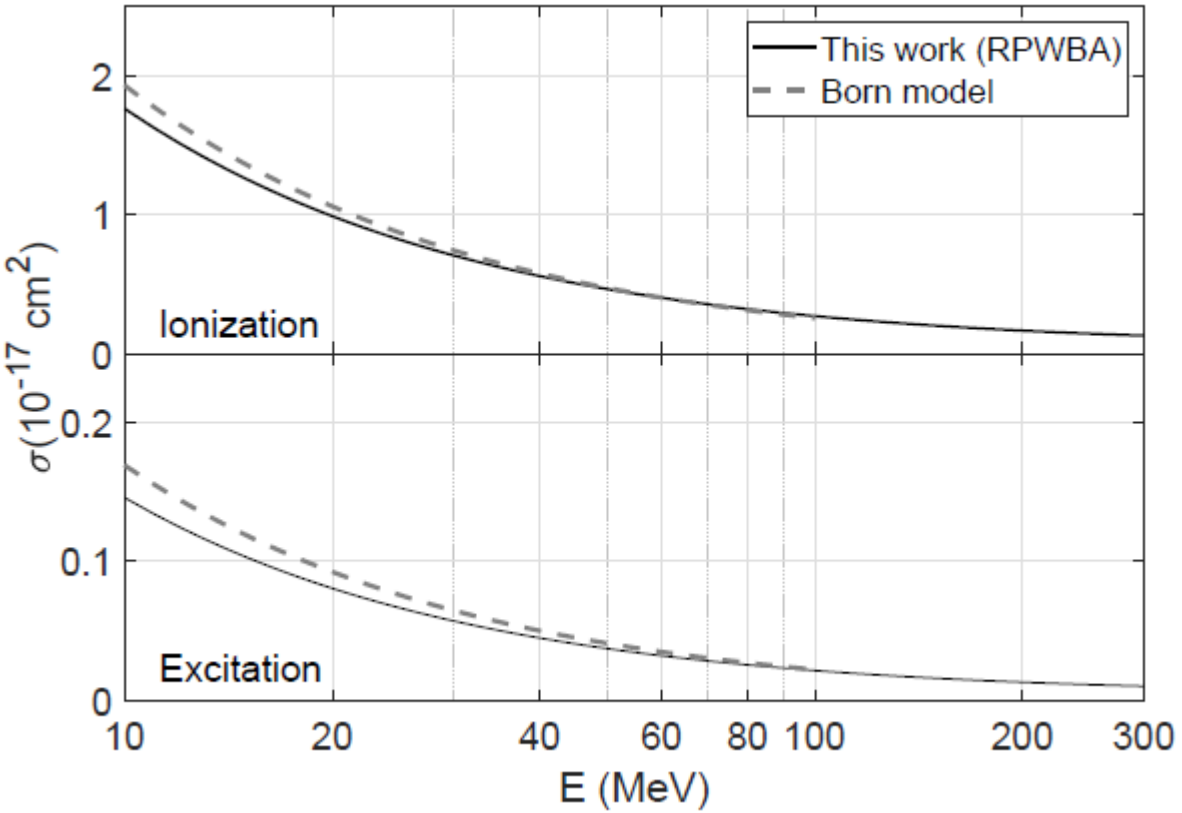
New data files from G4EMLOW8.1 → sigma_ionisation_p_RPWBA

RPWBA model verification

Ionisation DCS



Total CS



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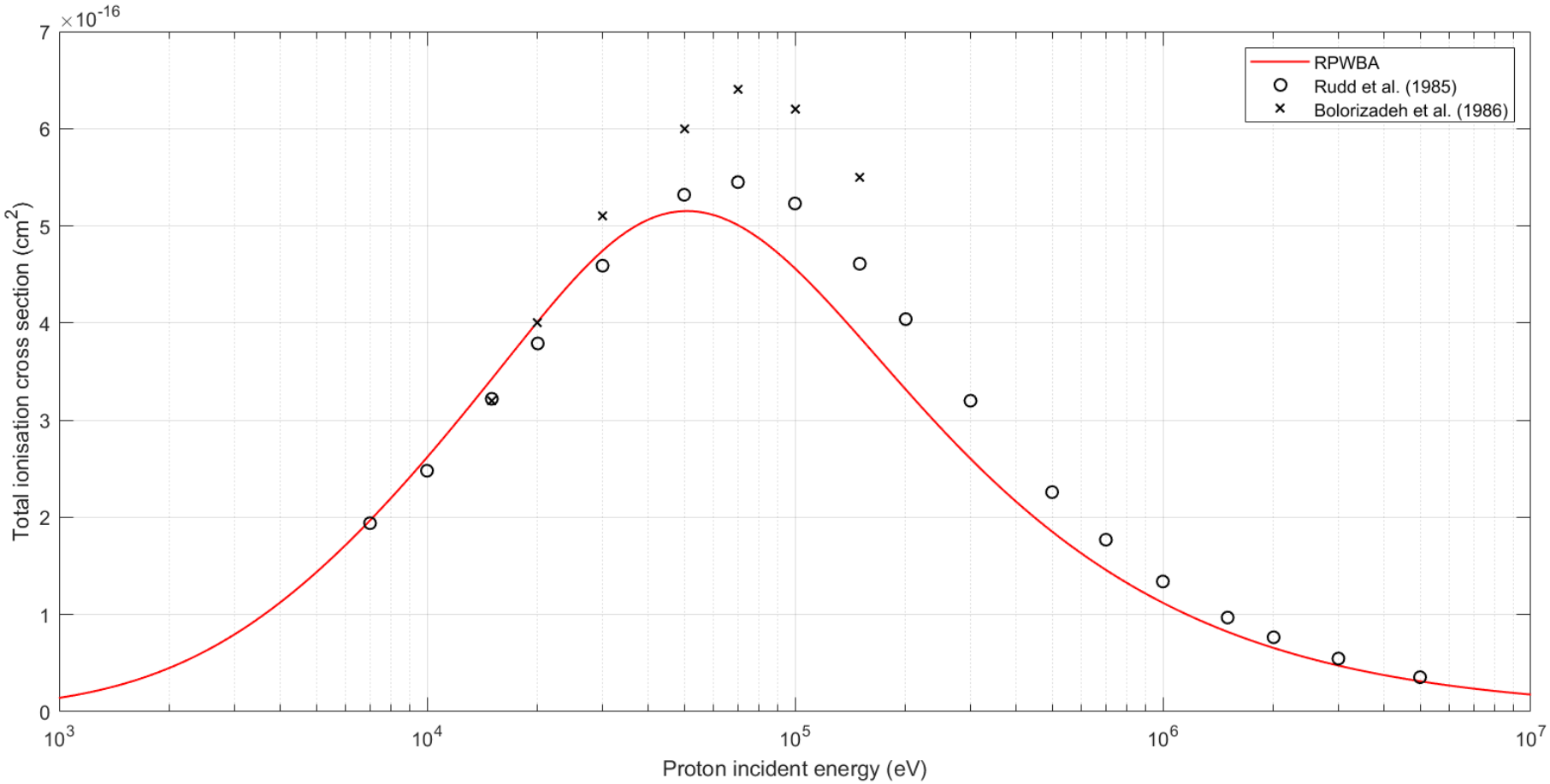
Validation of the model – Total Cross Section

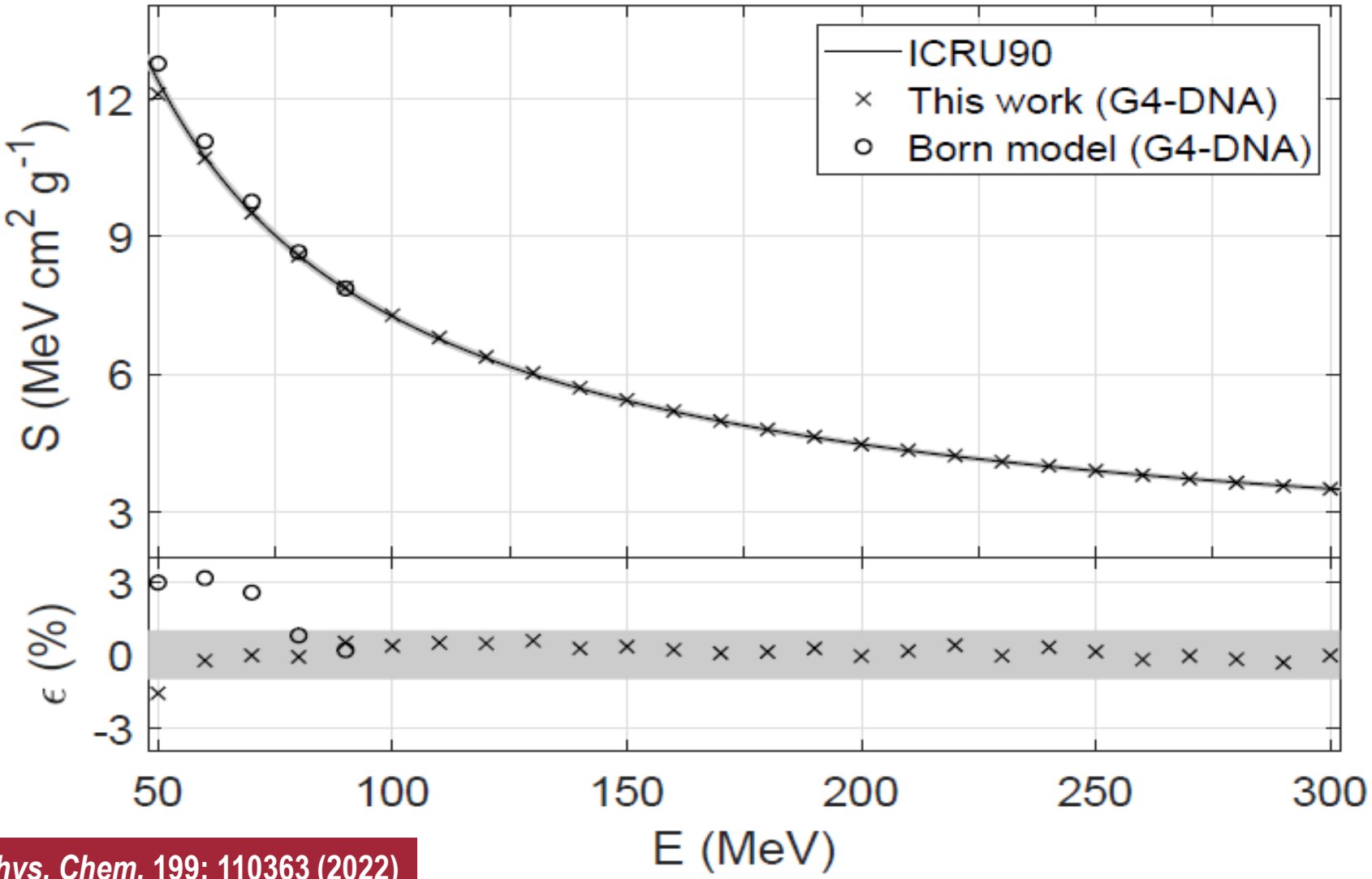
Ionisation CS

Experimental data for **vapour water**



Verification of the RPWBA code & database implementation

spower example



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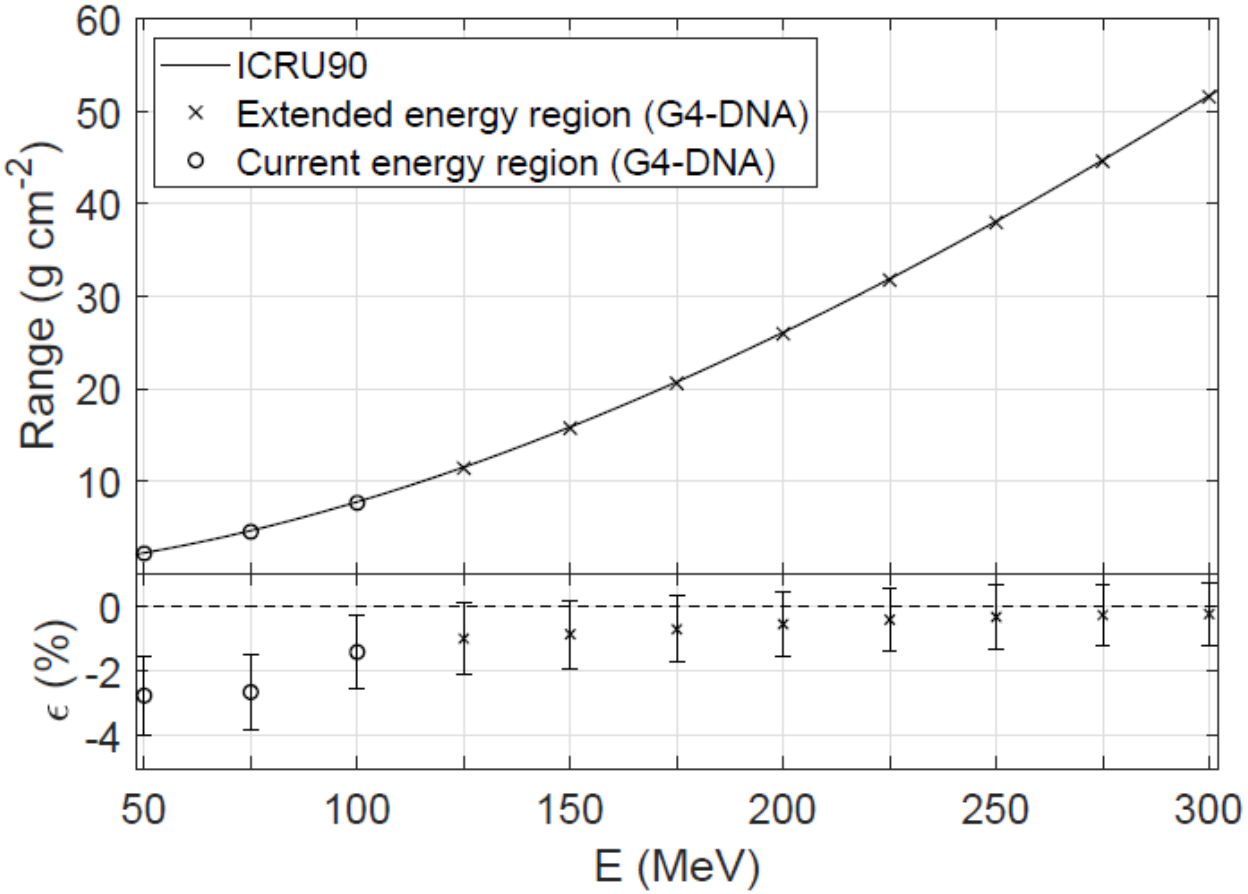
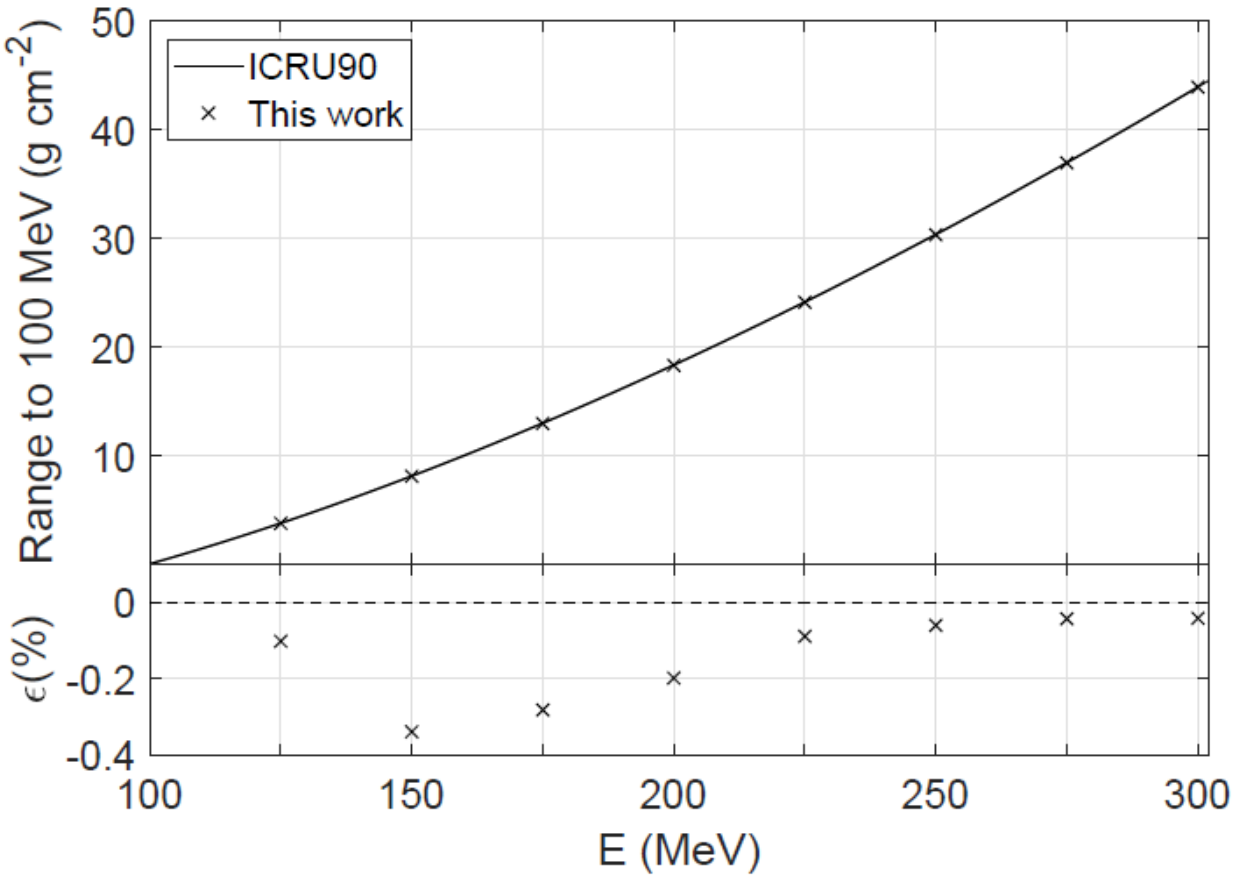
Verification of the RPWBA code & database implementation

range example

Transport down to zero energy



Transport down to 100 MeV



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Conclusions

- New G4DNA model available for protons **up to 300 MeV.**
  - The **entire range** of typical **proton therapy** energies is now covered.

- Maximum deviation w.r.t. existing Born model of 5% and 2%, ionization and excitation, respectively, for protons at 100 MeV.

- Agreement with ICRU90 values:
  - **spower:** within 1%.
  - **range:** within 0.5% for proton stopping above 100 MeV.

MORE INFO: A. D. Domínguez-Muñoz et al., *Radiat. Phys. Chem* 199: 110363 (2022) [https://doi.org/10.1016/j.radphyschem.2022.110363]

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