

Final implementation of RPWBA model in Geant4-DNA for proton transport up to 300 MeV

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IN2P3
Les deux infinis



27th Geant4 Collaboration Meeting

Rennes (France)

September 29th, 2022



Motivation and goal

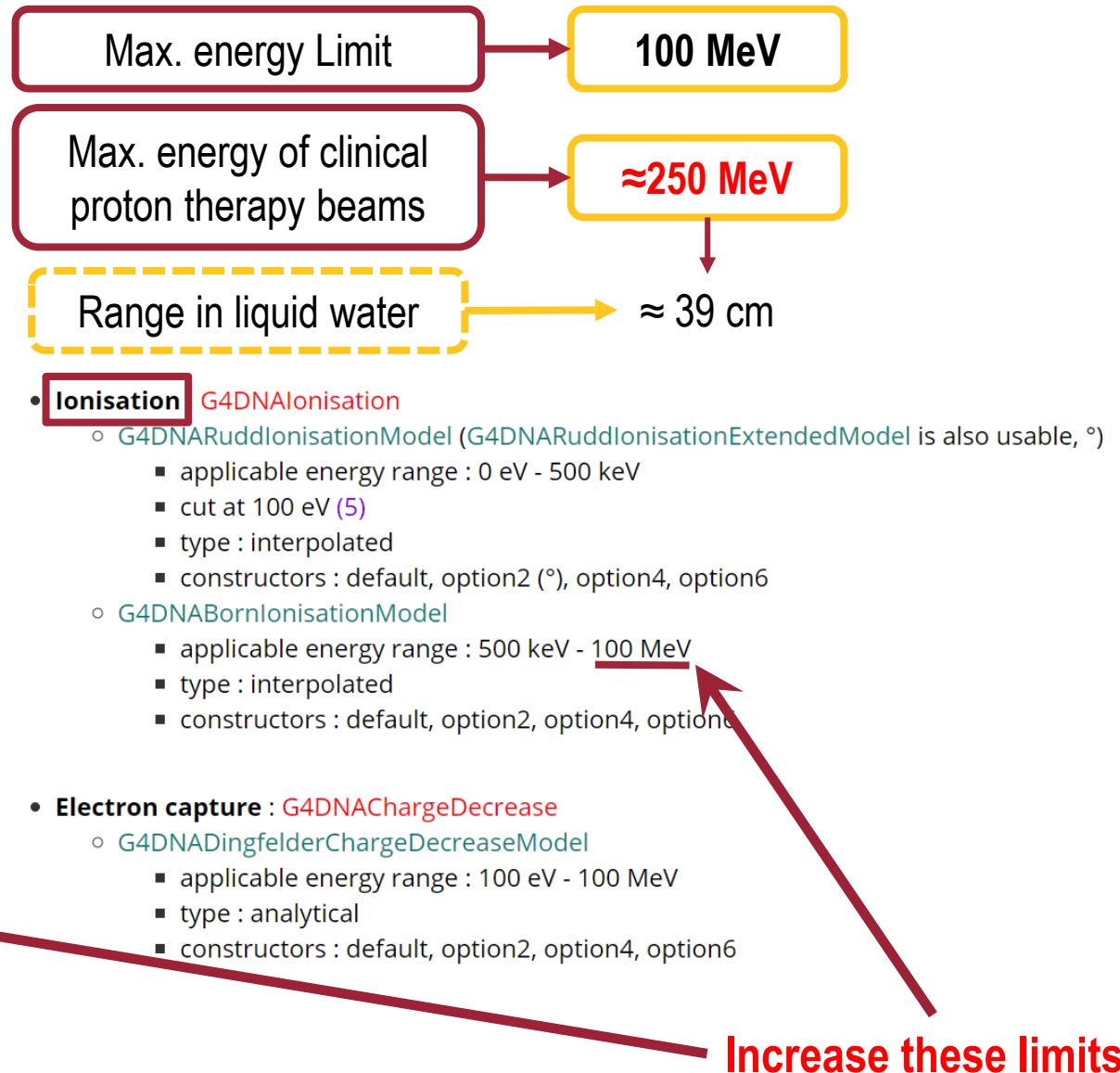


PROTONS (named "proton")

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

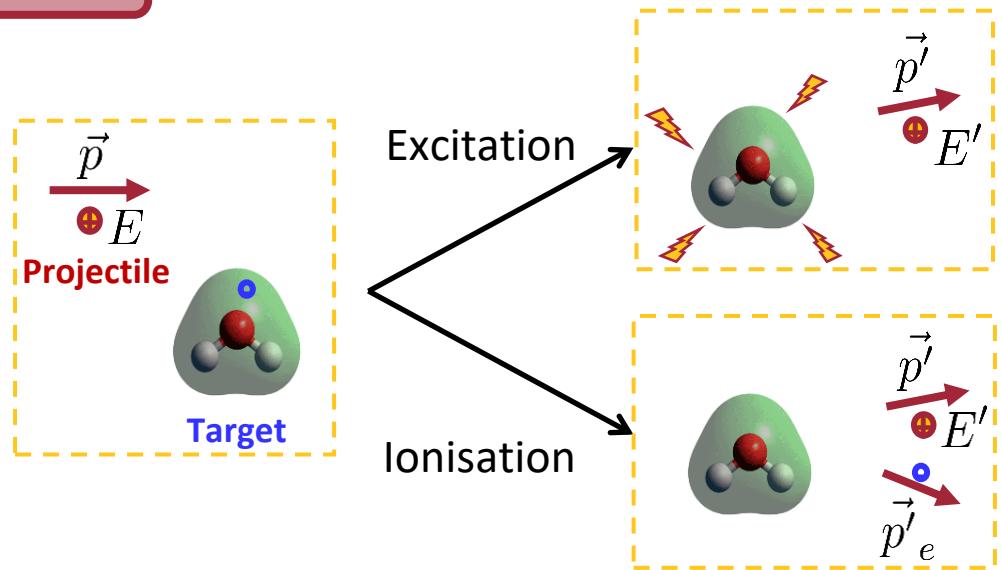


RPWBA Theory

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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

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

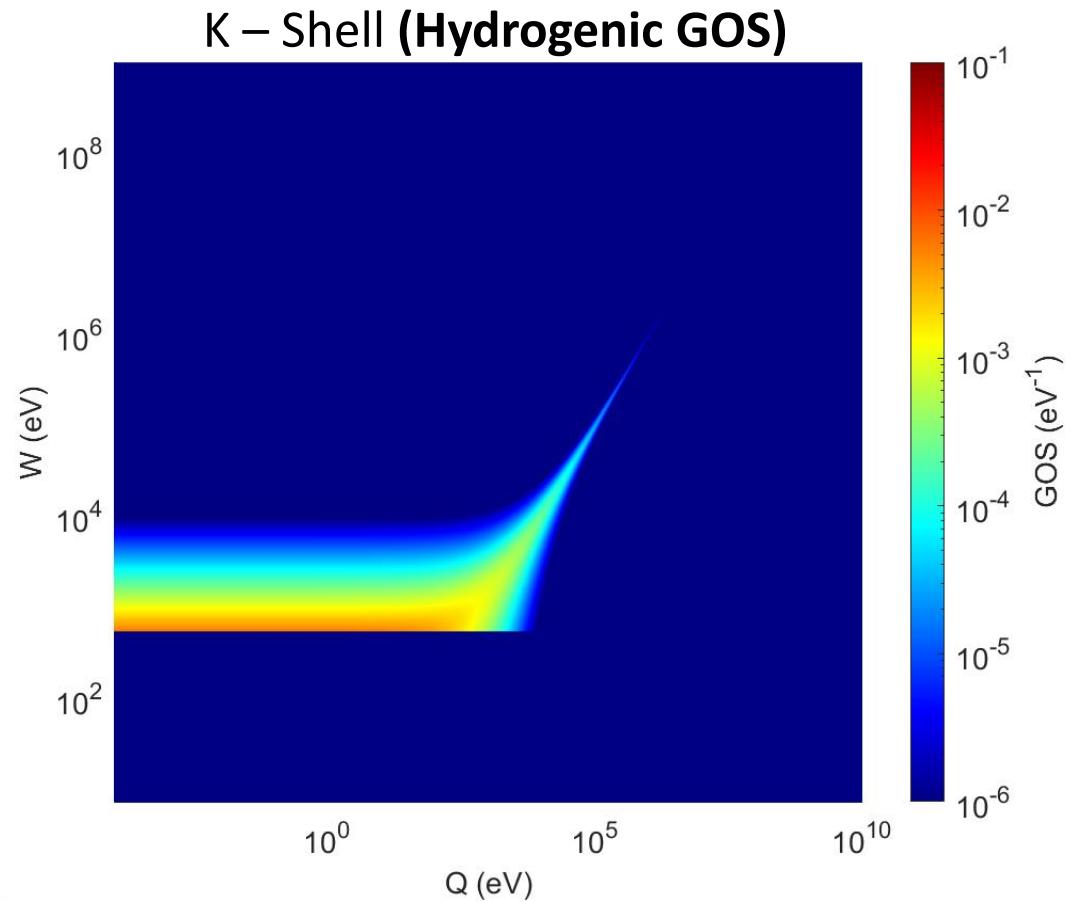
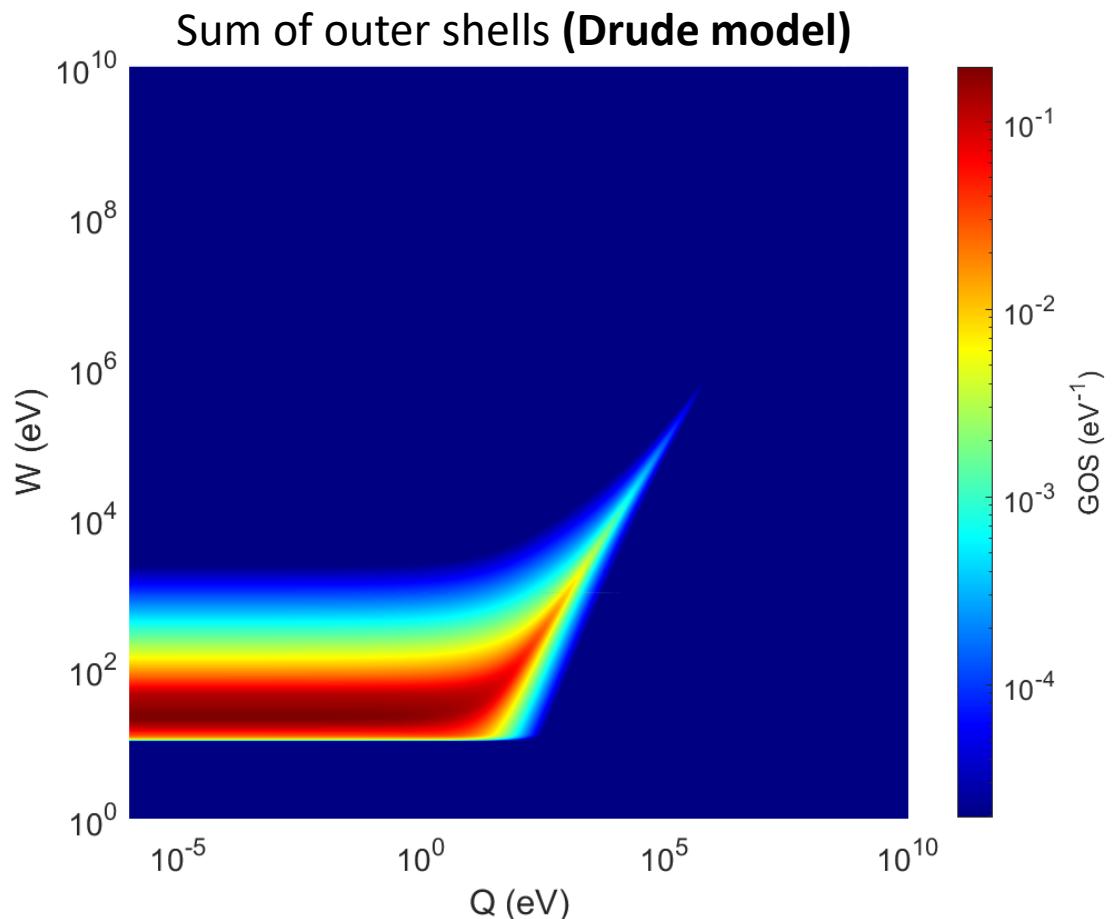
Generalized oscillator strength (GOS)

Response of the material

$$\frac{df(Q, W)}{dW}$$

Liquid Water GOS

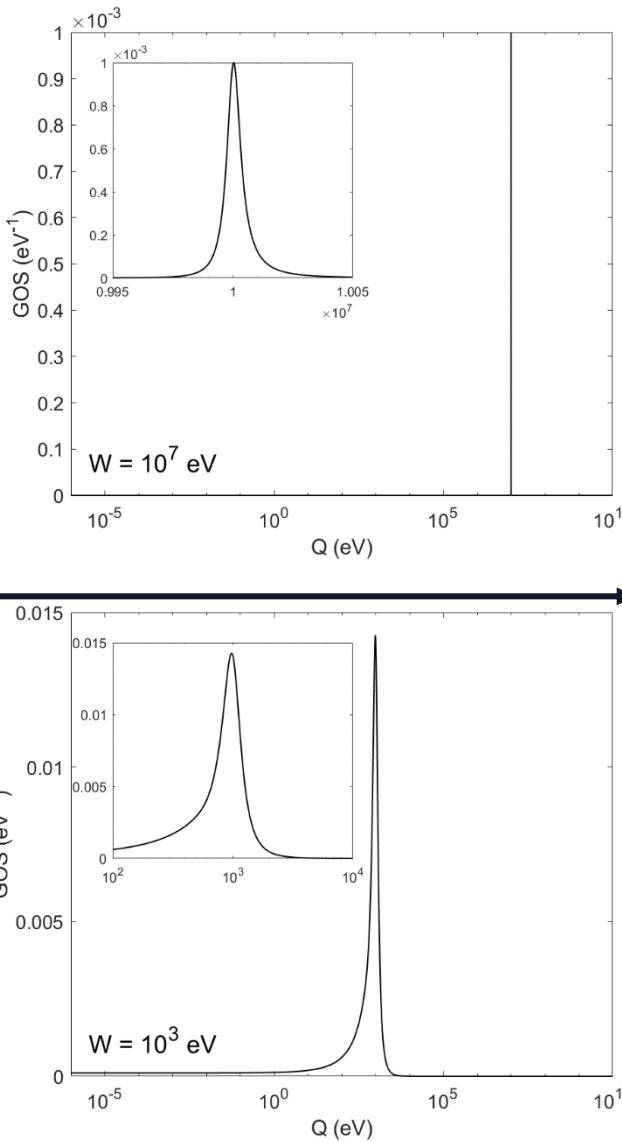
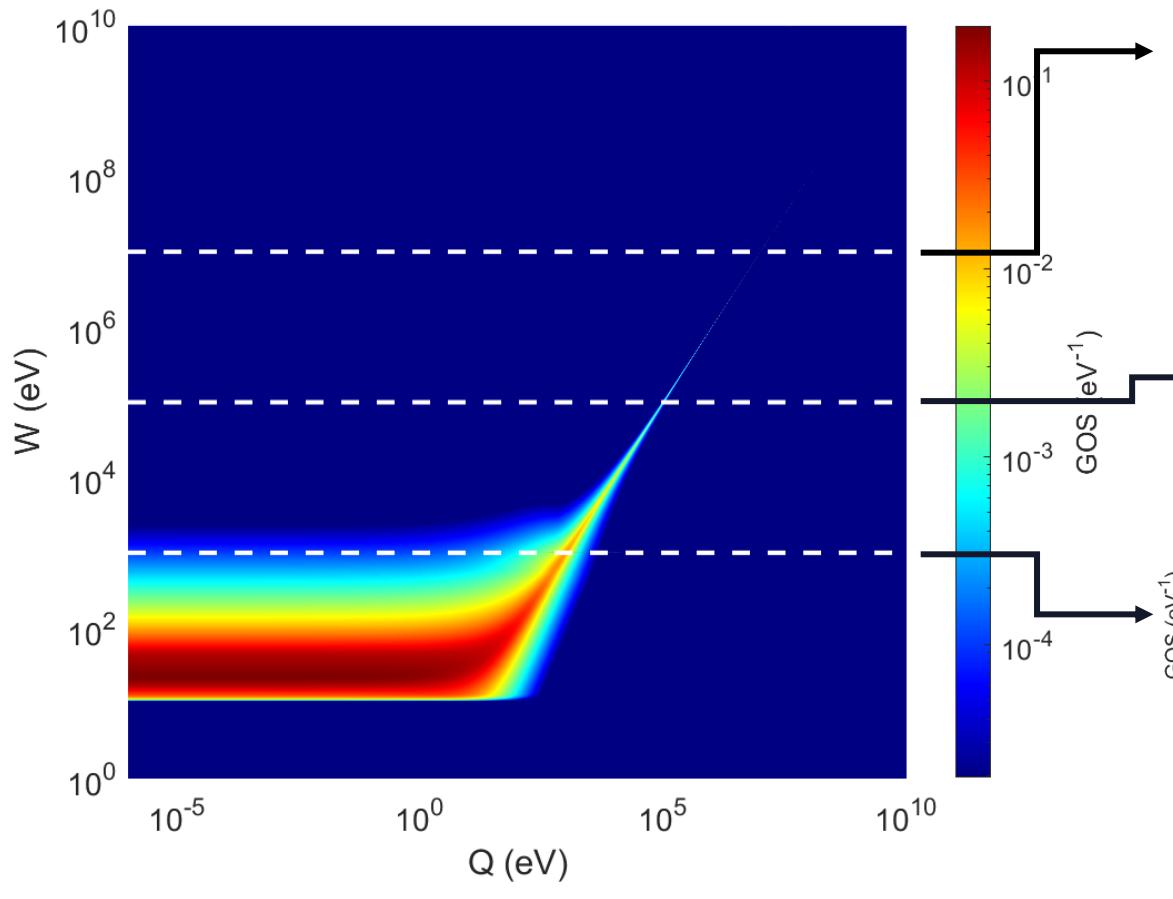
Ionisation GOS



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

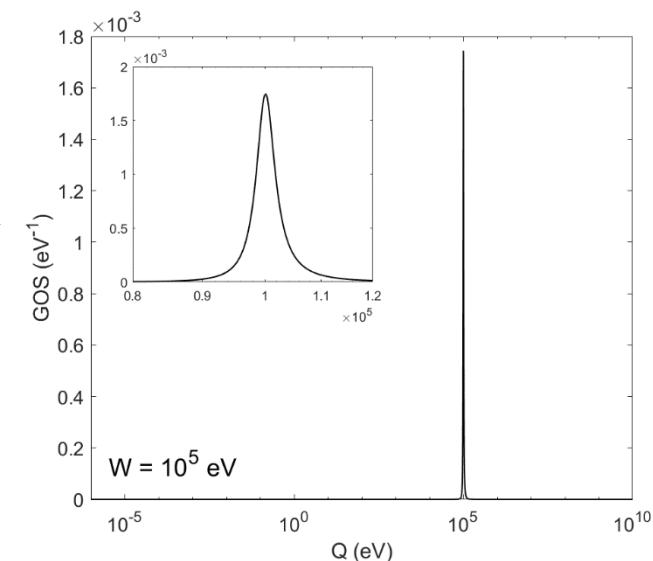
Liquid Water GOS

Ionisation GOS



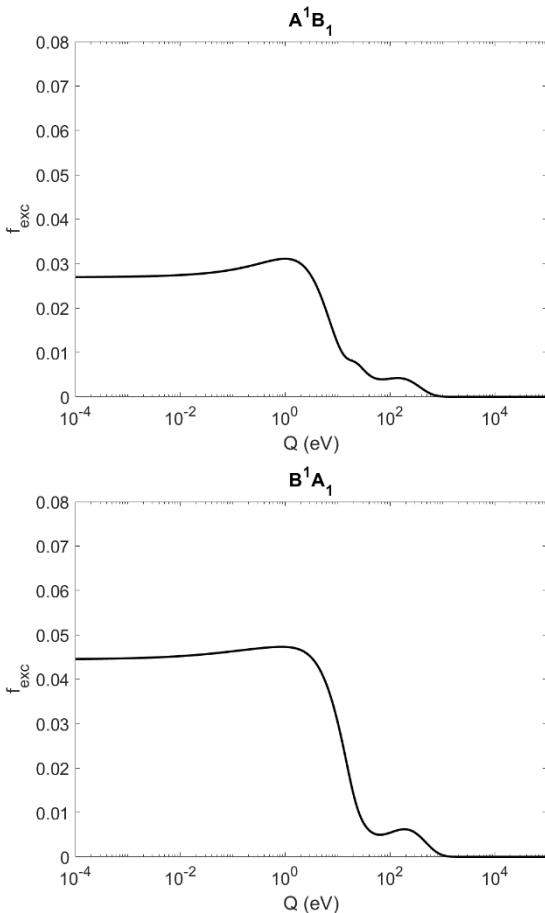
Adaptative grid to
reproduce numerically the
Bethe-Ridge accurately

Necessary for numerical
integration of DDCS



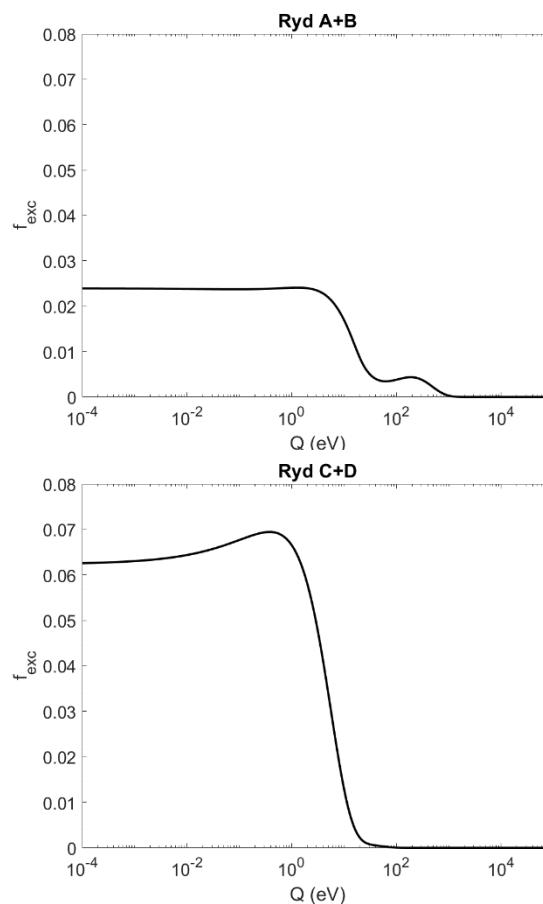
Liquid Water GOS

Excitation GOS



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

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

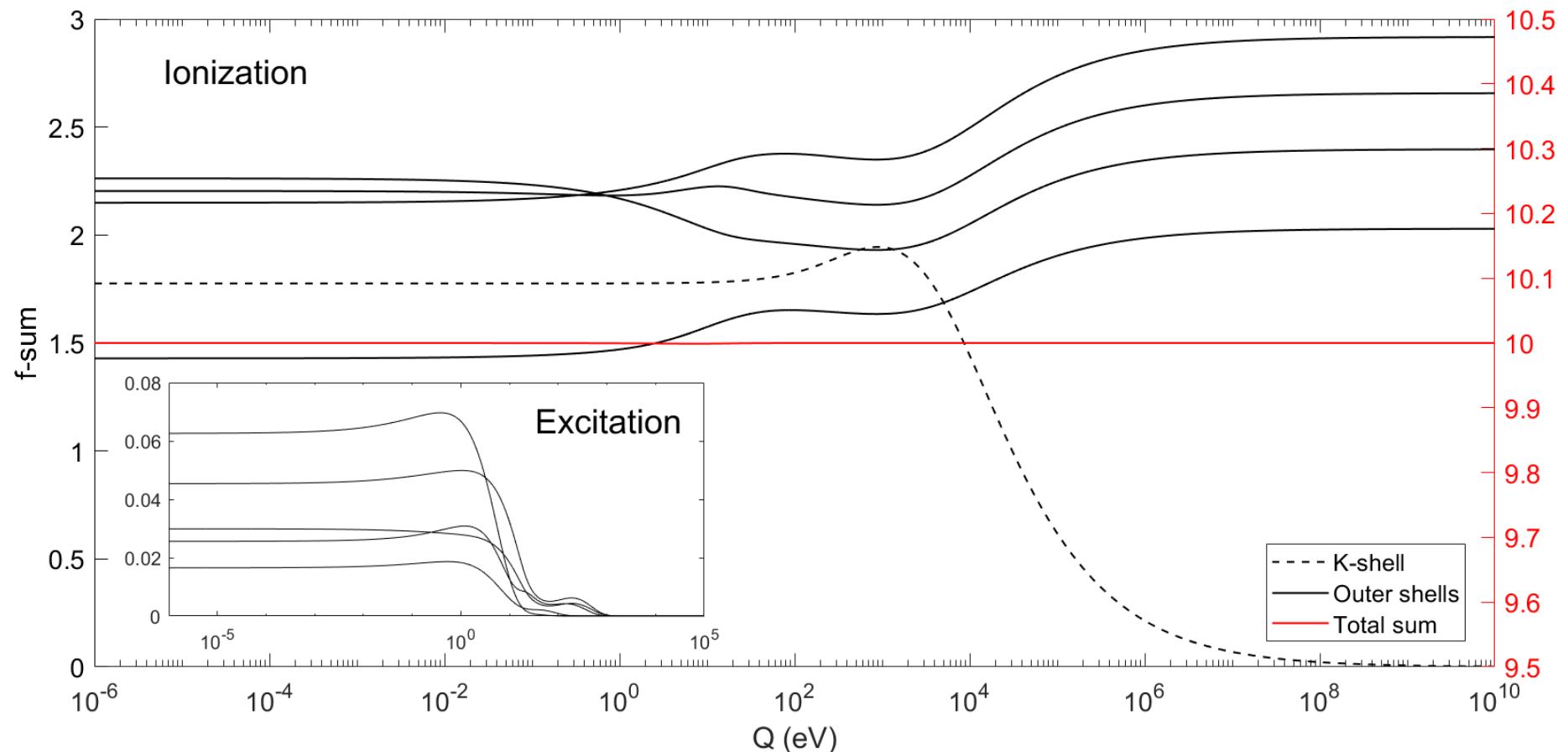
[D. Emfietzoglou / *Radiation Research* 164 (2005) 202–211]

Liquid Water GOS

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GOS properties

I -value = 77.955 eV



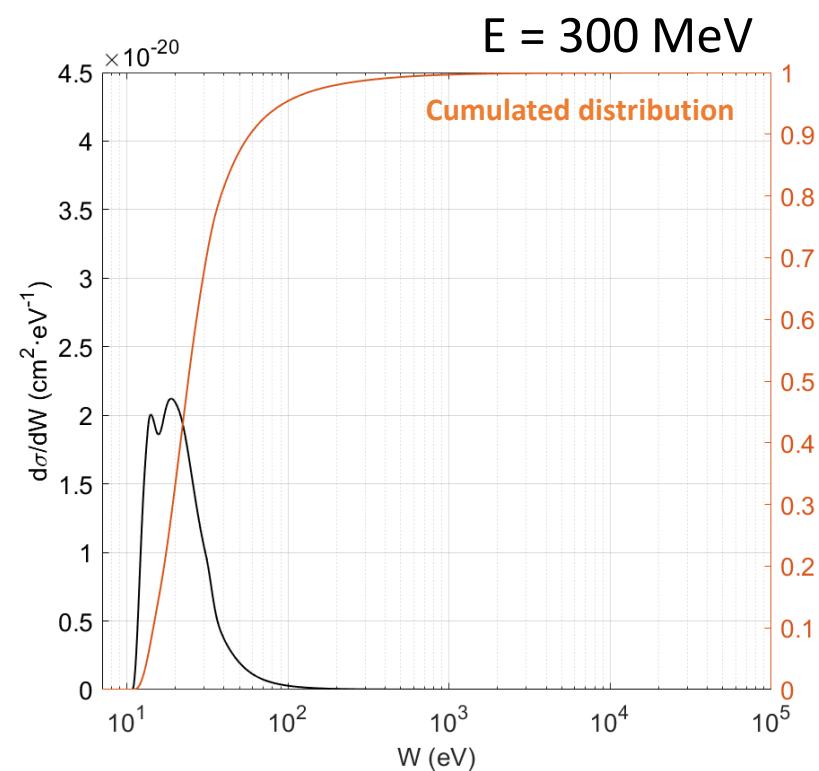
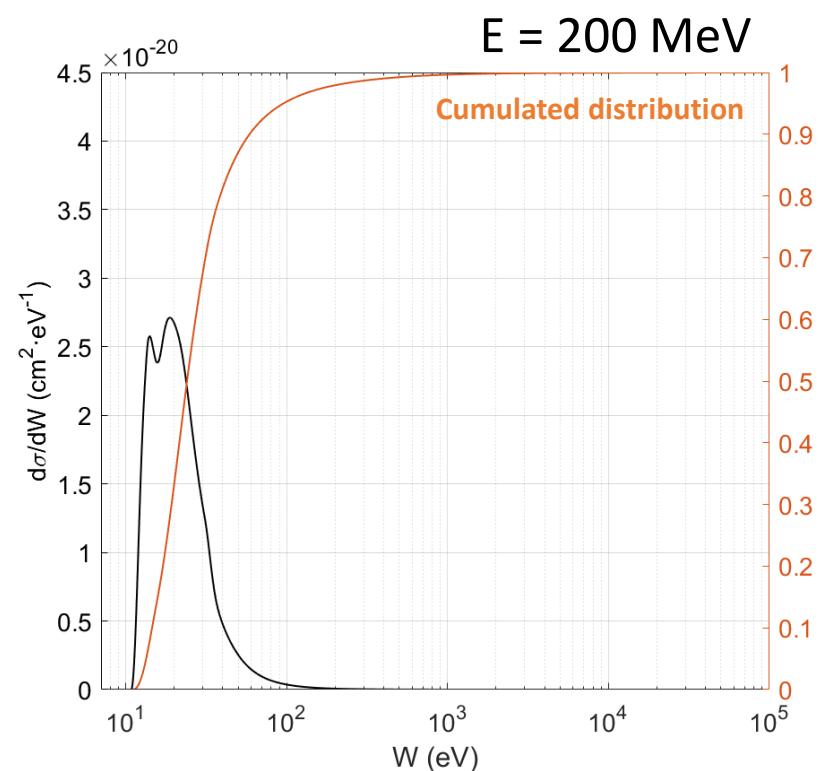
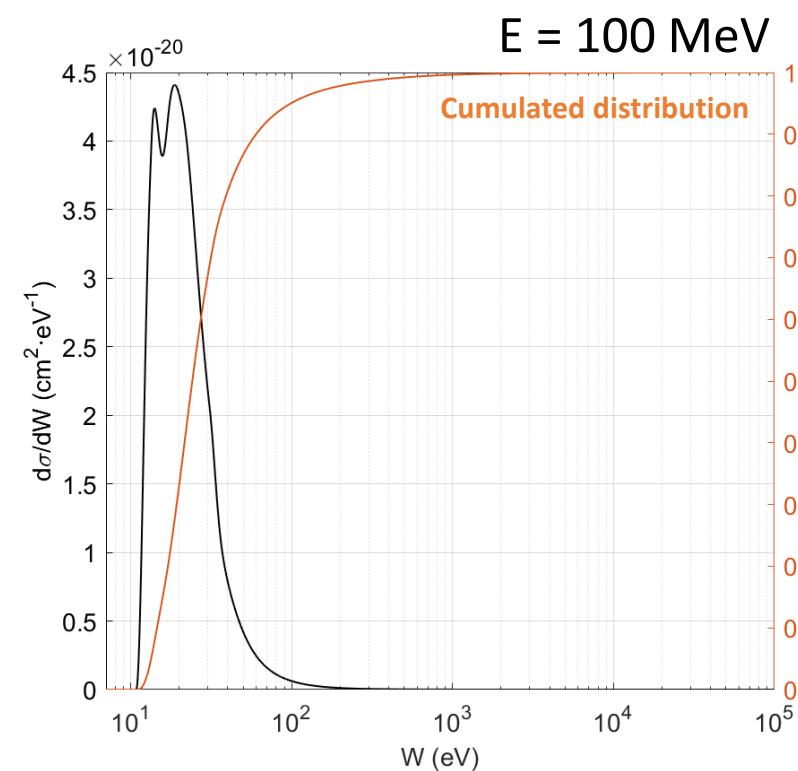
Calculation of datasets

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

1b₁ - shell

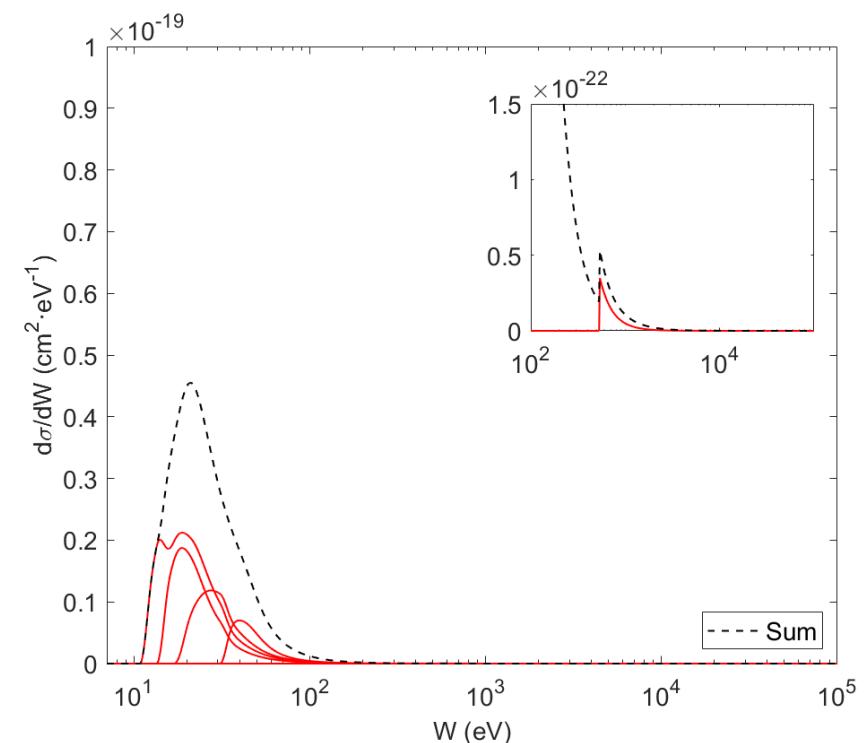
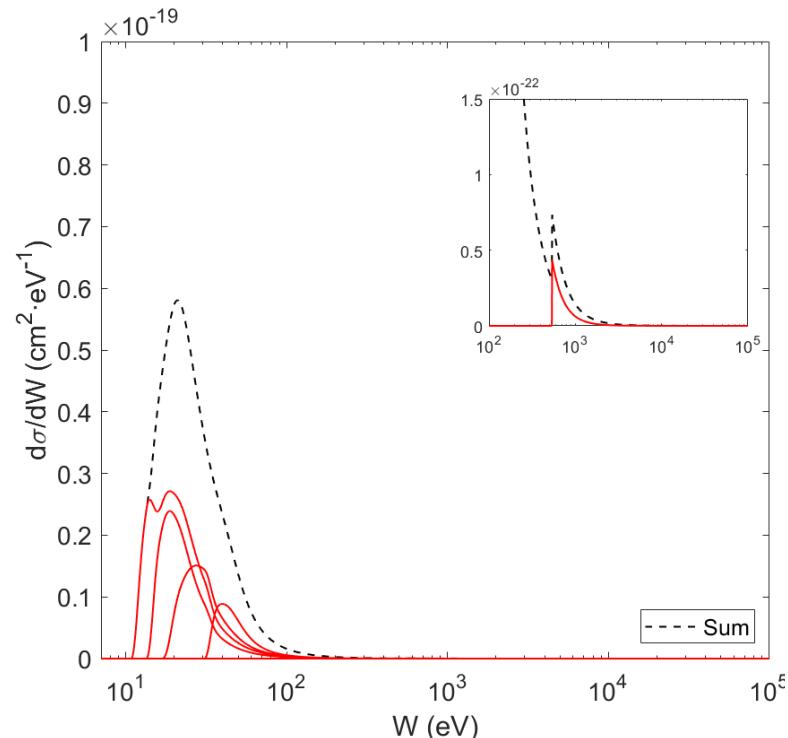
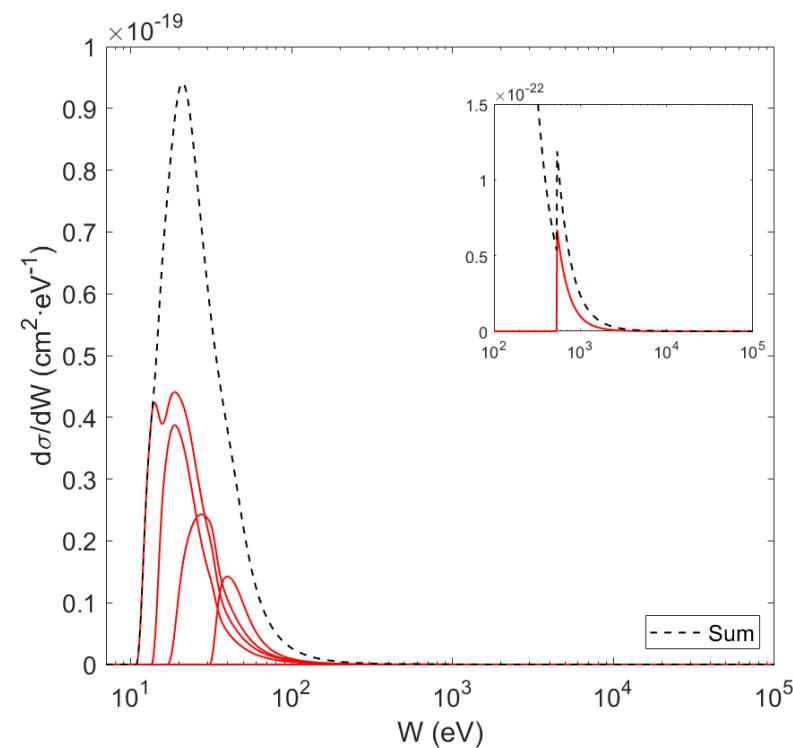


Calculation of datasets

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



New data files from G4EMLOW8.1 →

sigmadiff_ionisation_p_RPWBA

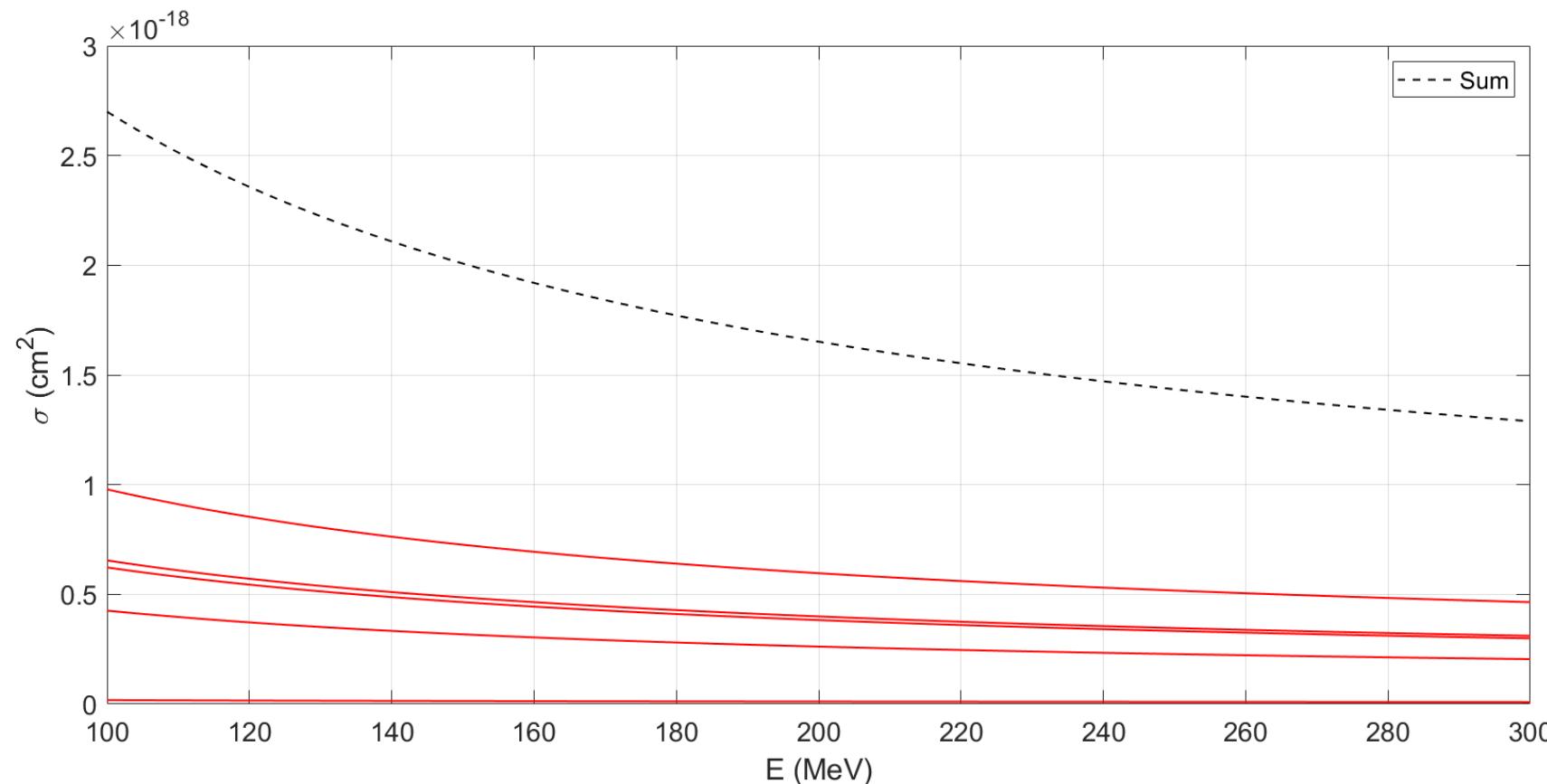
sigmadiff_cumulated_ionisation_p_RPWBA

Calculation of datasets

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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

New RPWBA classes within G4DNA models

-  G4DNARPWBAExcitationModel.cc
-  G4DNARPWBAlonisationModel.cc

-  G4DNAExcitation.cc
-  G4DNAIonisation.cc

Models

Processes

Available already in gitlab →

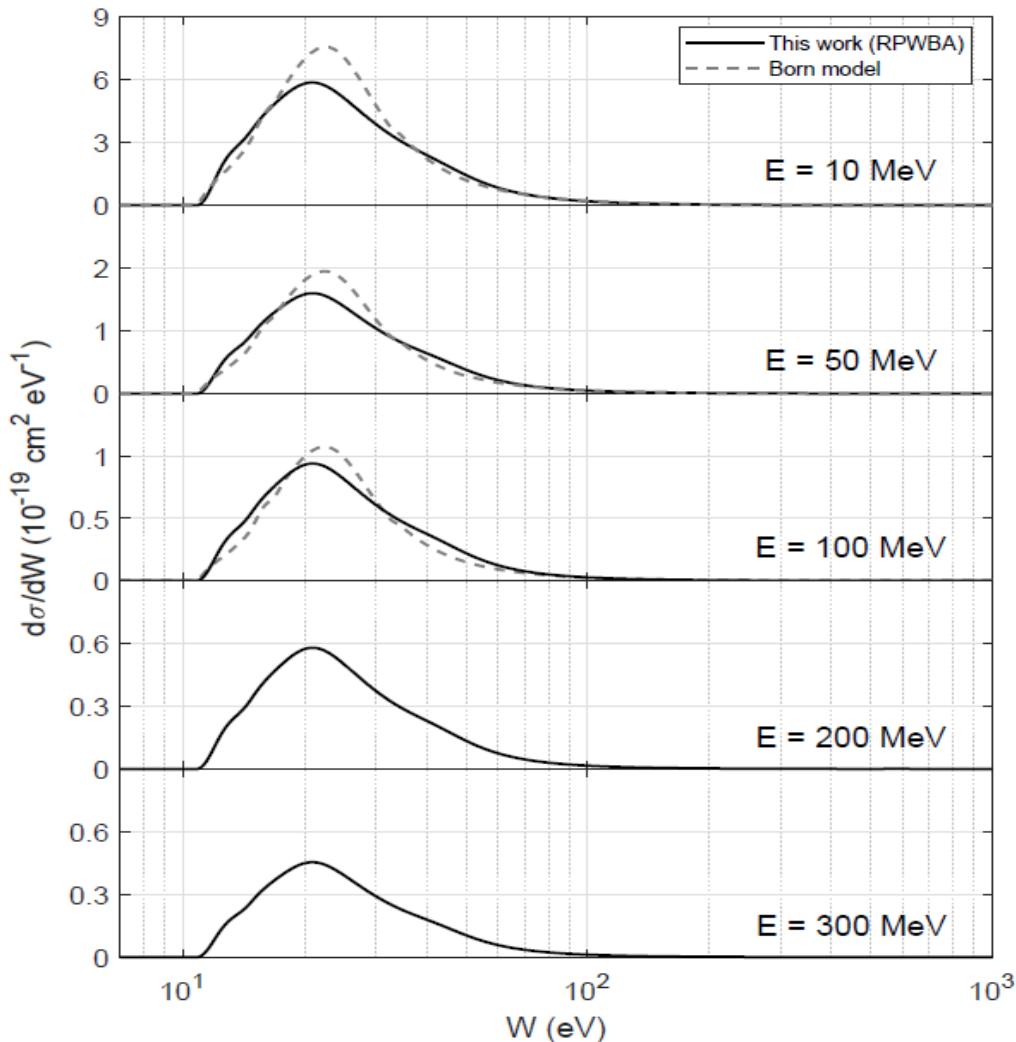
Implementation analogous to
G4DNABorn models

 G4DNAMolecularStepByStepModel.cc	[clean][timeboxed] chemistry	3 years ago
 G4DNASequenceStepper.cc	IRT classes w clear master branch	2 years ago
 G4DNAOneStepThermalizationModel.cc	removal of cout	2 years ago
 G4DNAPTBAugerModel.cc	correct permissions to 664 for files with extension .cc, .hh...	1 year ago
 G4DNAPTBELasticModel.cc	Replace getenv() calls for data variables with G4FindData...	4 months ago
 G4DNAPTBExcitationModel.cc	correct permissions to 664 for files with extension .cc, .hh...	1 year ago
 G4DNAPTBIonisationModel.cc	Replace getenv() calls for data variables with G4FindData...	4 months ago
 G4DNAQuinnPlasmonExcitationModel.cc	emdna-V11-00-23, use G4FindDataDir(G4LEDATA) to find...	3 months ago
 G4DNARPWBAExcitationModel.cc	Updated reference paper of DNA RPWBA model classes	4 weeks ago
 G4DNARPWBAlonisationModel.cc	Updated reference paper of DNA RPWBA model classes	4 weeks ago
 G4DNARelativisticIonisationModel.cc	emdna-V11-00-23, use G4FindDataDir(G4LEDATA) to find...	3 months ago
 G4DNA RuddAngle.cc	removed cvs keywords	3 years ago
 G4DNA RuddIonisationExtendedModel.cc	correct DNA ion definition	3 months ago
 G4DNA RuddIonisationModel.cc	DNA code optimization:	5 months ago
 G4DNA SanchezExcitationModel.cc	emdna-V11-00-23, use G4FindDataDir(G4LEDATA) to find...	3 months ago
 G4DNA ScreenedRutherfordElasticModel.cc	fixed coverity warnings	2 years ago
 G4DNA SmoluchowskiDiffusion.cc	changed files during release checks, i.e. update of math f...	6 years ago
 G4DNA SmoluchowskiReactionModel.cc	Optimize IRT-syn model, delete G4DNAIRI_geometries	7 months ago
 G4DNA TransformElectronModel.cc	removed cvs keywords	3 years ago
 G4DNA UeharaScreenedRutherfordElasticM...	fix coverity warning	2 years ago

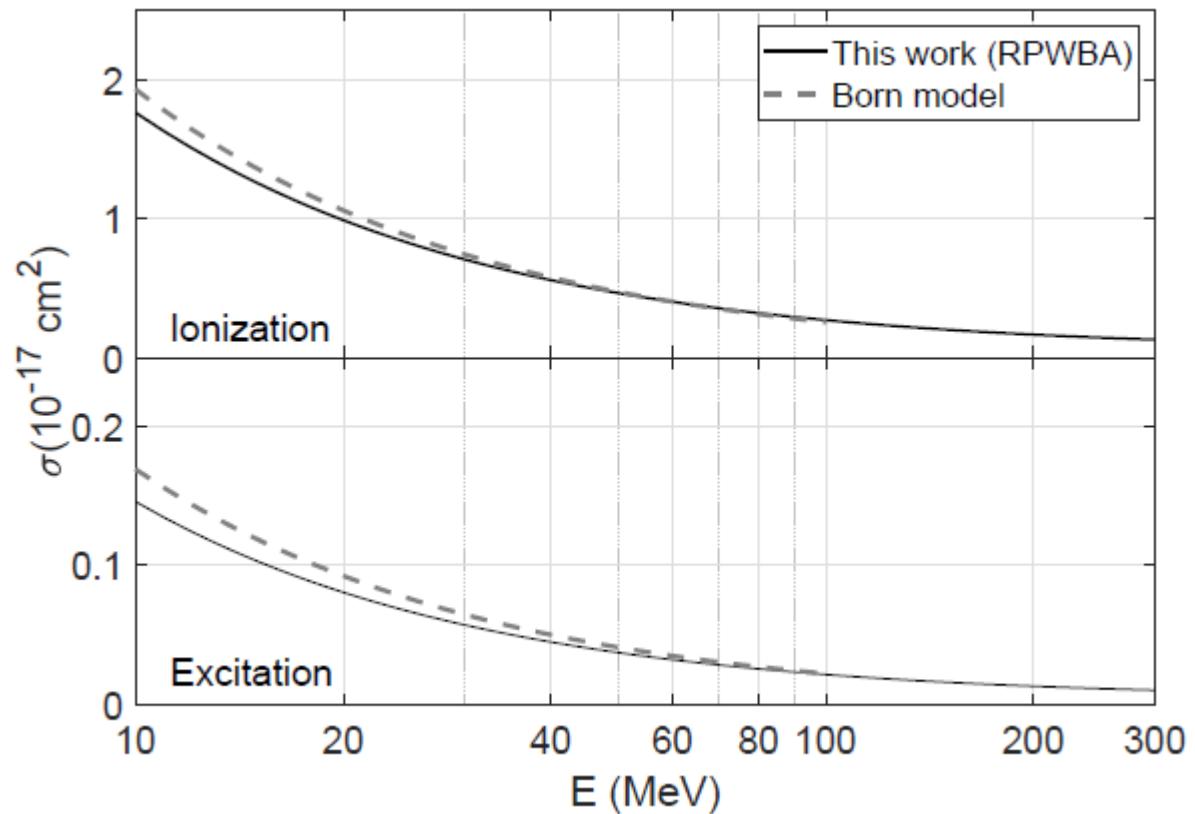
RPWBA model verification

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Ionisation DCS



Total CS

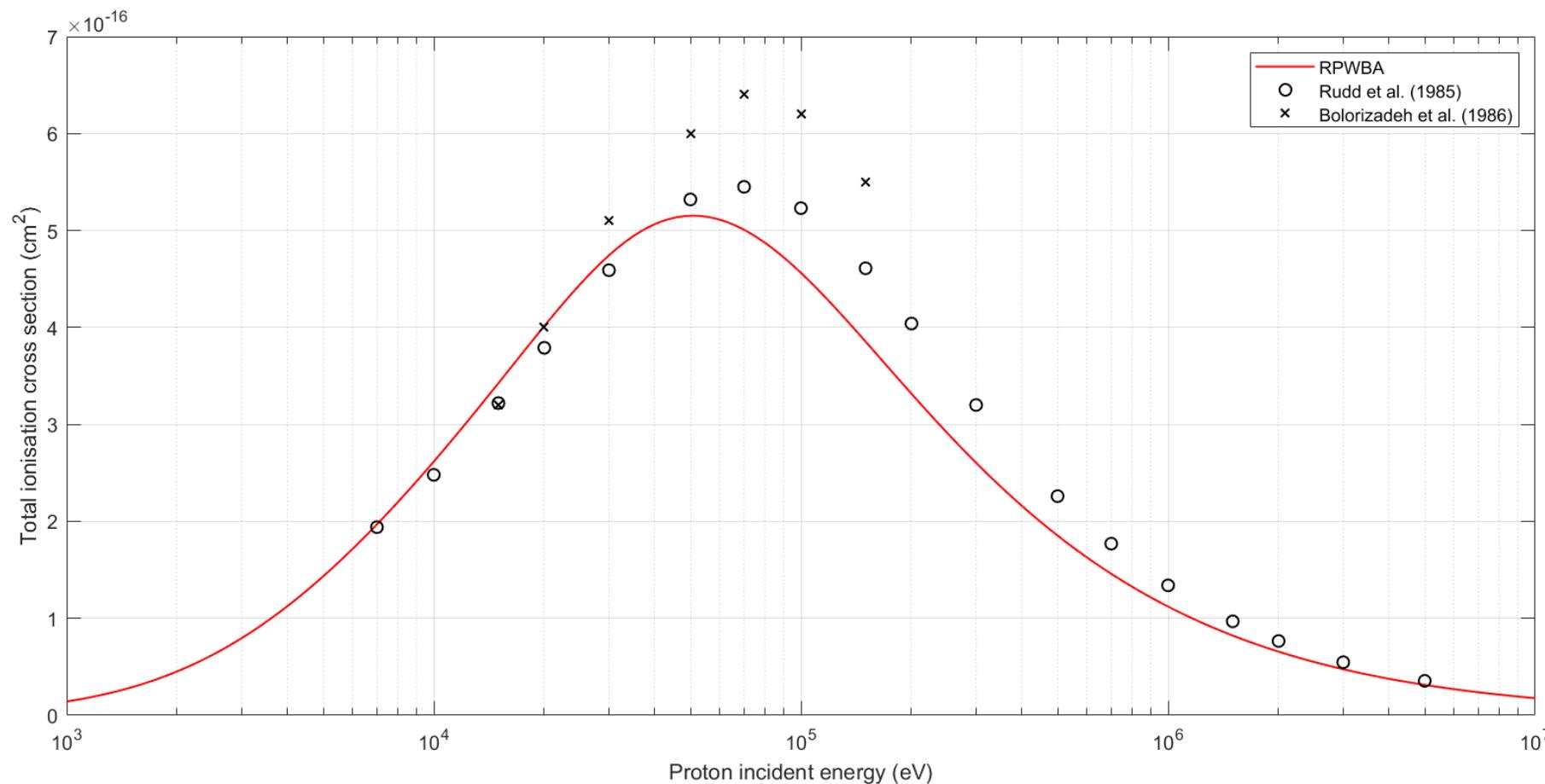


Validation of the model – Total Cross Section

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Ionisation CS

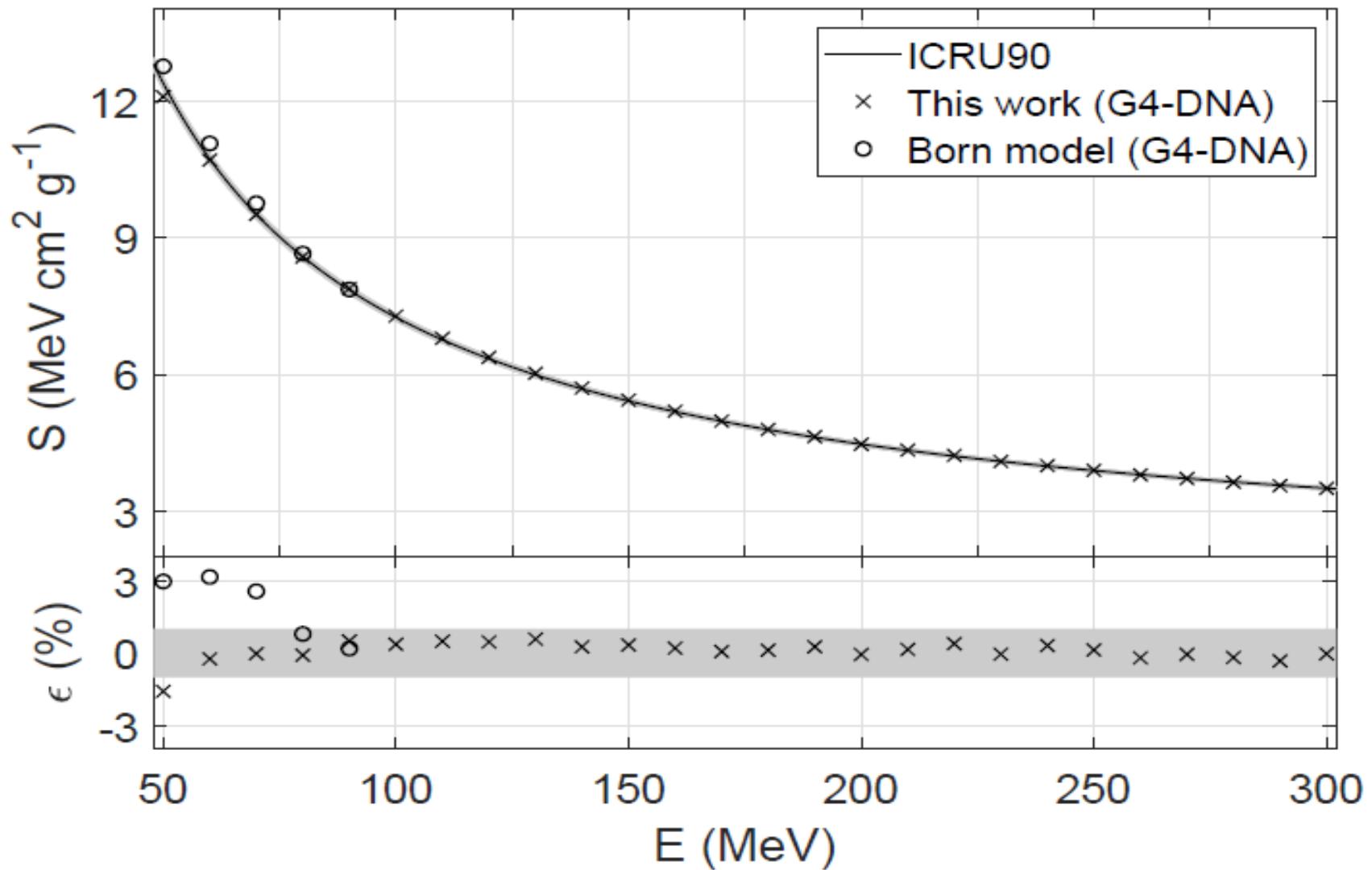
Experimental data for **vapour water**



Verification of the RPWBA code & database implementation

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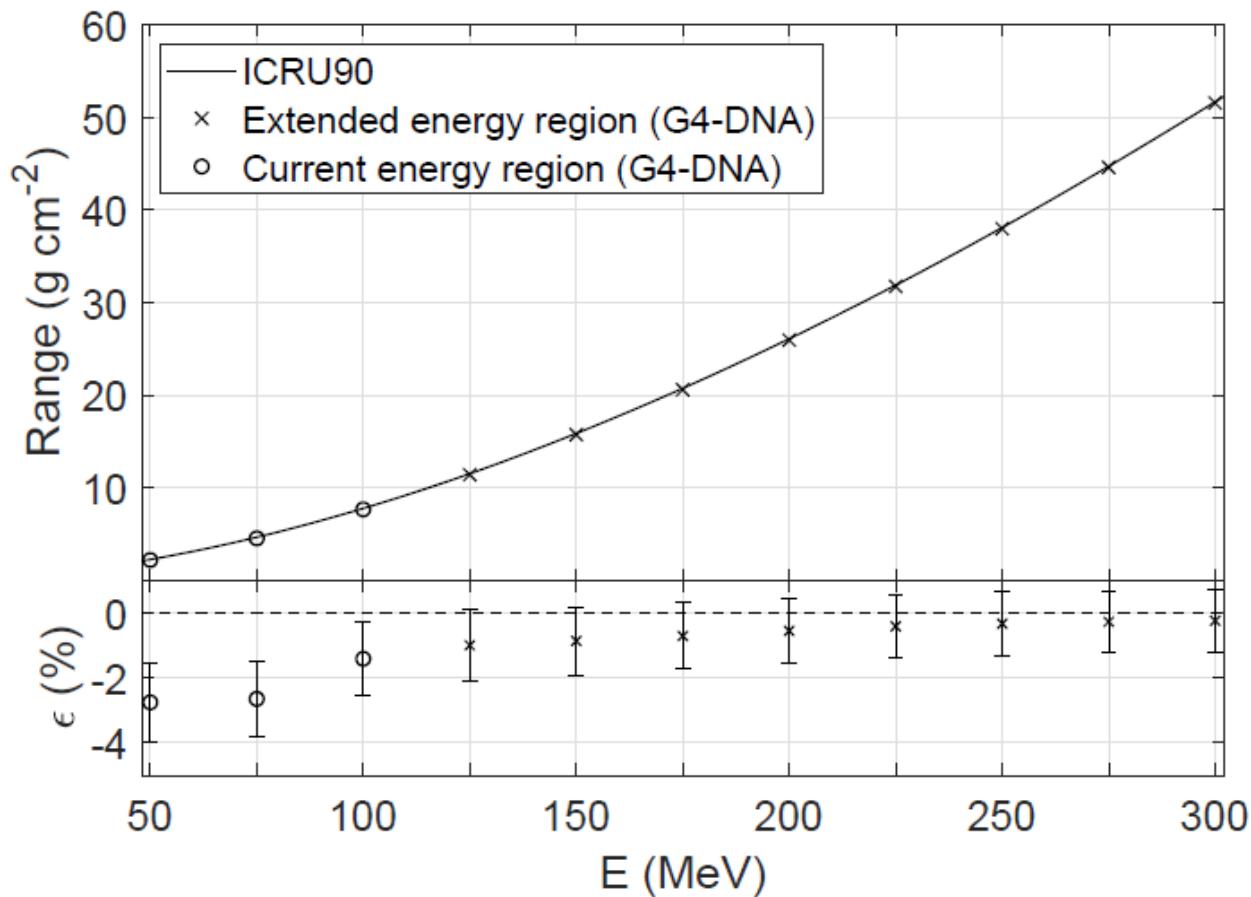
spower example



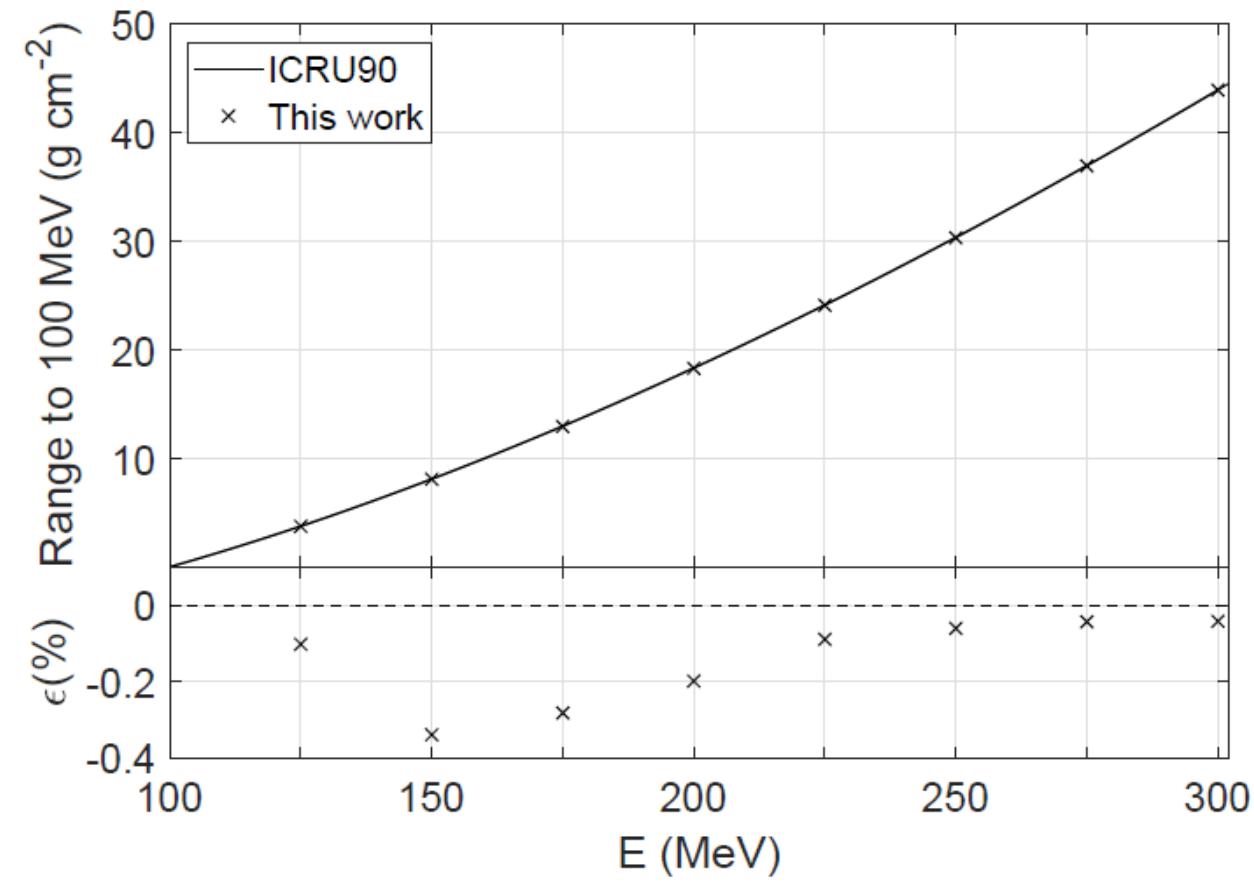
Verification of the RPWBA code & database implementation

range example

Transport down to zero energy



Transport down to 100 MeV



Conclusions

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- 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:
 - **s_{power}**: 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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