Covering the upper clinical energy range of Geant4-DNA for proton transport in liquid water

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Outline

- Motivation and goal
- Theoretical framework: RPWBA
- GOS of liquid water
- Results
- Conclusions and future work

Motivation and goal

GEANT4-DNA
A SIMULATION TOOLKIT

http://geant4-dna.org/

Max. energy Limit → 100 MeV

Max. energy of clinical proton therapy beams → ≈250 MeV → ≈ 39 cm

Range in liquid water → ≈ 39 cm

- **Proton interactions** **Liquid water**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill (5)	Type
nuclear scattering (5)	G4DNAElastic	G4DNAIonElasticModel	100 eV	1 MeV	100 eV	interpolated
electronic excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	10 eV	500 keV	-	analytical
electronic excitation	G4DNAExcitation	G4DNABornExcitationModel	500 keV	100 MeV	-	interpolated
ionisation	G4DNAIonisation	G4DNARuddIonisationModel (G4DNARuddIonisationExtendedModel is also usable)	0 eV	500 keV	100 eV	interpolated
ionisation	G4DNAIonisation	G4DNABornIonisationModel	500 keV	100 MeV	-	interpolated
electron capture	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	100 eV	100 MeV	-	analytical

(5) indicates the tracking cut applied by the corresponding model.

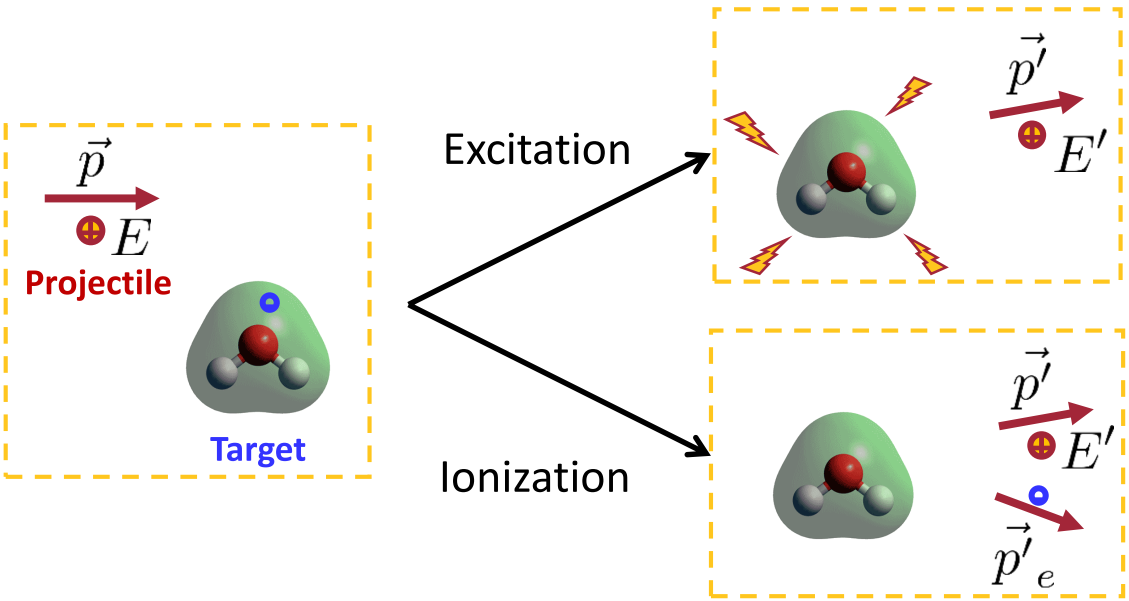
Theoretical framework: RPWBA

RPWBA **Relativistic Plane Wave Born Approximation**

Relativistic Quantum Mechanics Dirac equation

Projectile $\mathcal{H}_P$ | Interaction $\mathcal{H}_{int}$ | Target $\mathcal{H}_T$

First Order Perturbation



Interaction hamiltonian

Two terms (Fano 1963)
- Longitudinal
- Transversal

Plane Wave Approximation — Initial and final projectile wavefunction → Free particle states (plane wave)

Theoretical framework: RPWBA

RPWBA **Relativistic Plane Wave Born Approximation**

Individual inelastic collisions

Characterized by

Energy loss $W = E - E'$

Momentum transfer $\vec{q} = \vec{p} - \vec{p'}$ → Recoil energy Q

DDCS **Doubly differential cross section** (E>>W)

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

Generalized oscillator strength

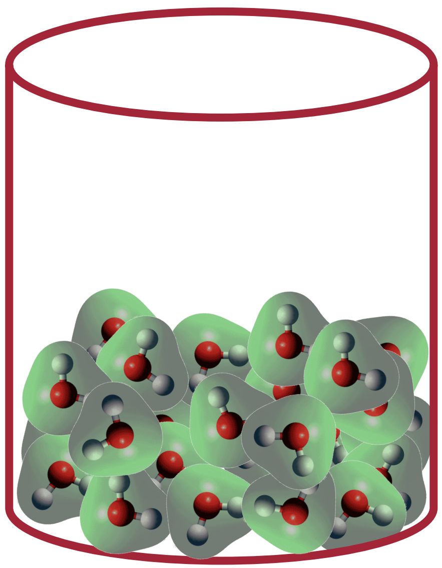
Response of the material

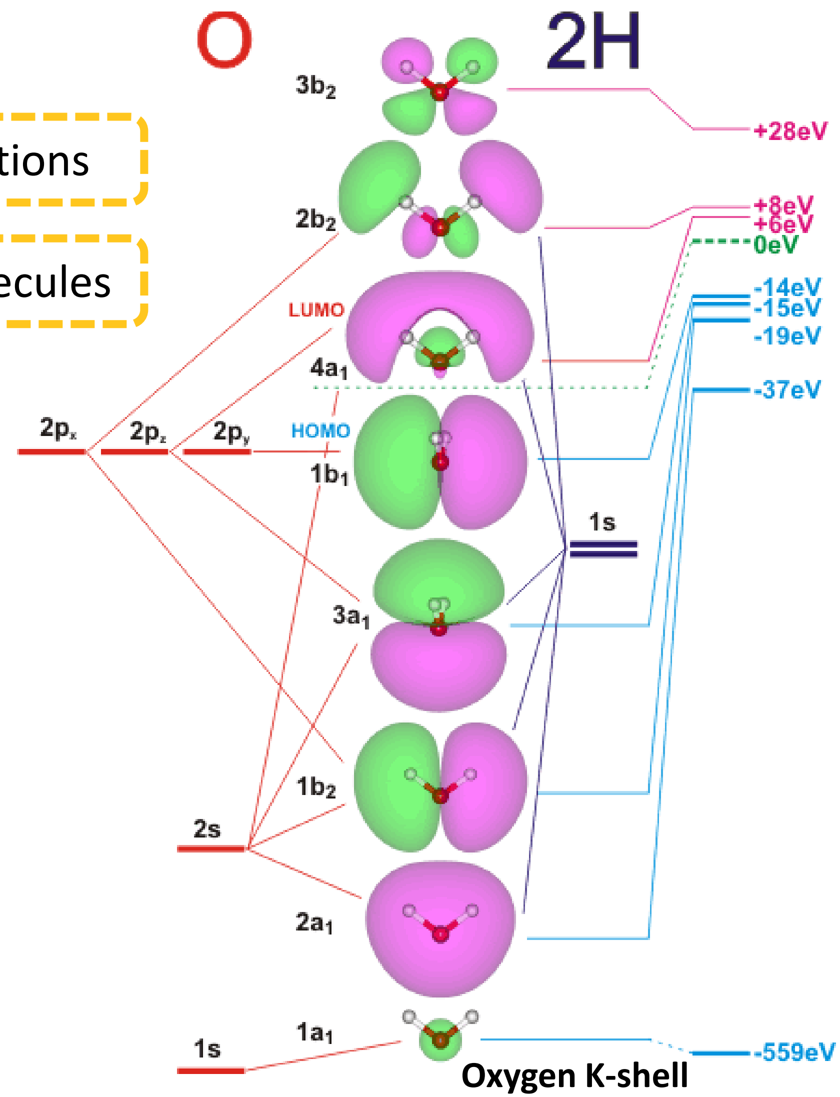
$\frac{df(Q,W)}{dW}$ **GOS??** $\frac{dg(Q,W)}{dW}$ **TGOS??**

GOS of liquid water

Difficulties of computing liquid water GOS

Molecule	Non spherical wavefunctions
Condensed phase	Interaction between molecules





GOS of liquid water

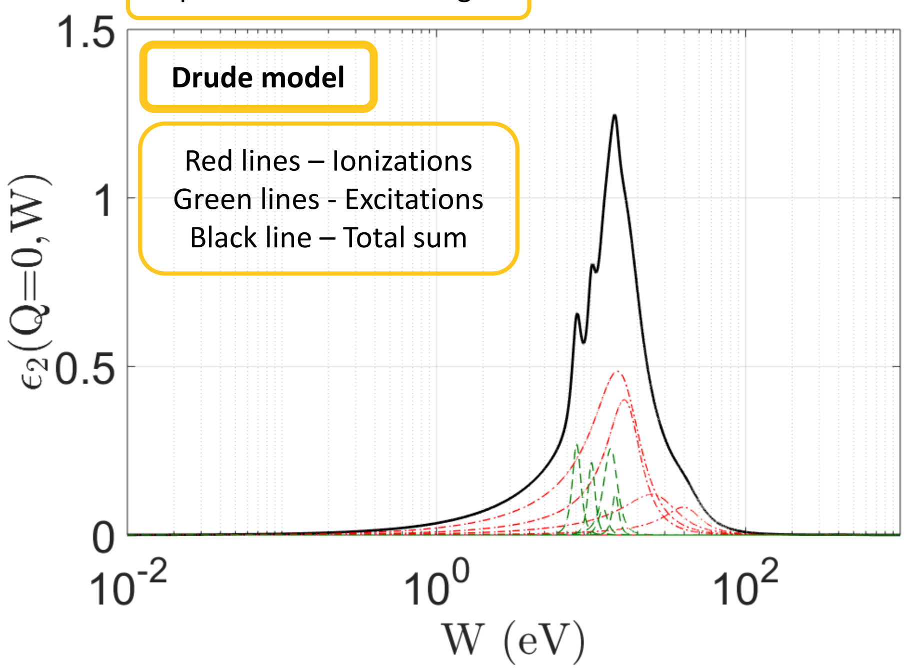
Connecting GOS with dielectric properties

GOS can be calculated from dielectric functions

[M. Dingfelder / *Radiation Physics and Chemistry 53 (1998) 1-18*]

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

Optical Oscillator Strength



Parameters values taken from

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

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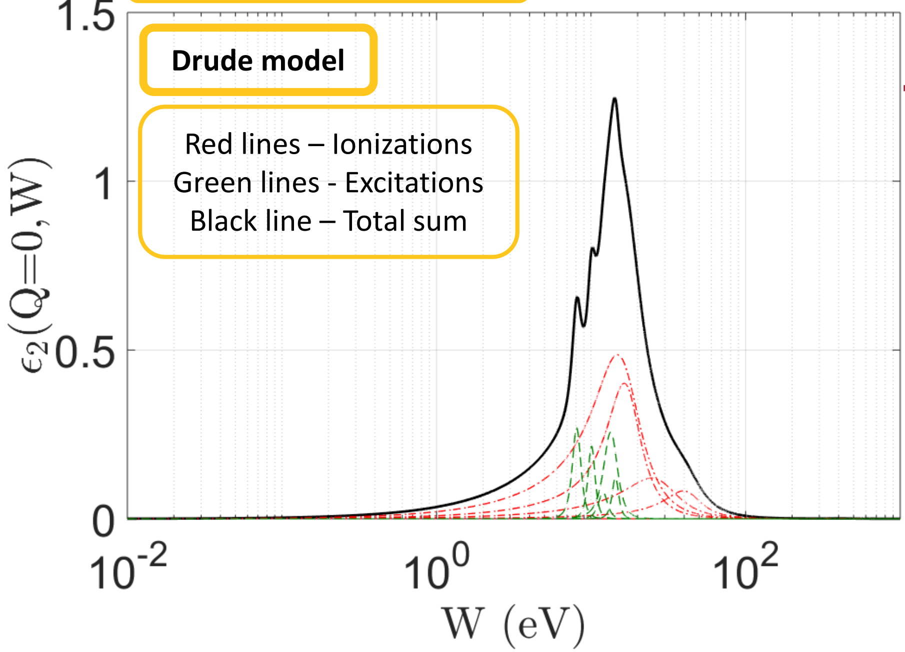

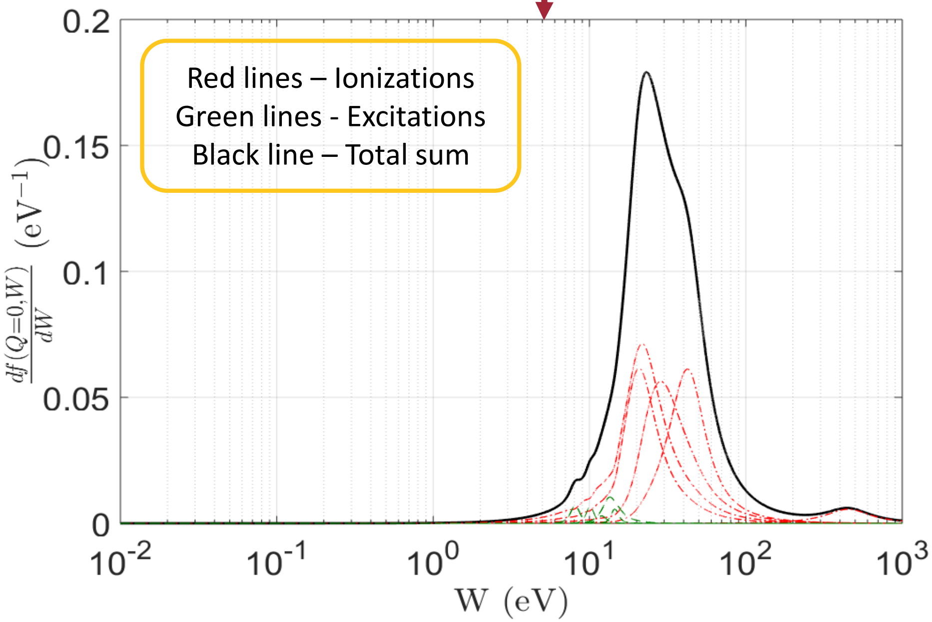

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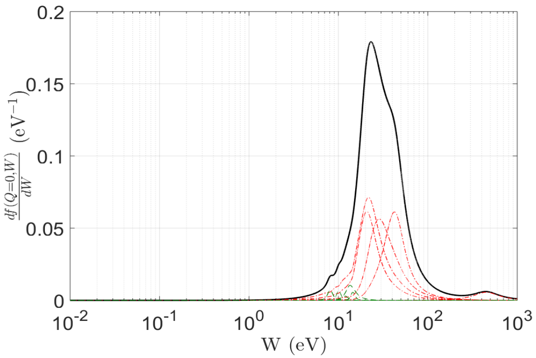
Q=0



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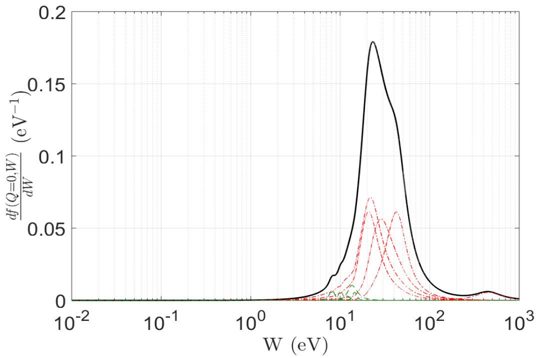
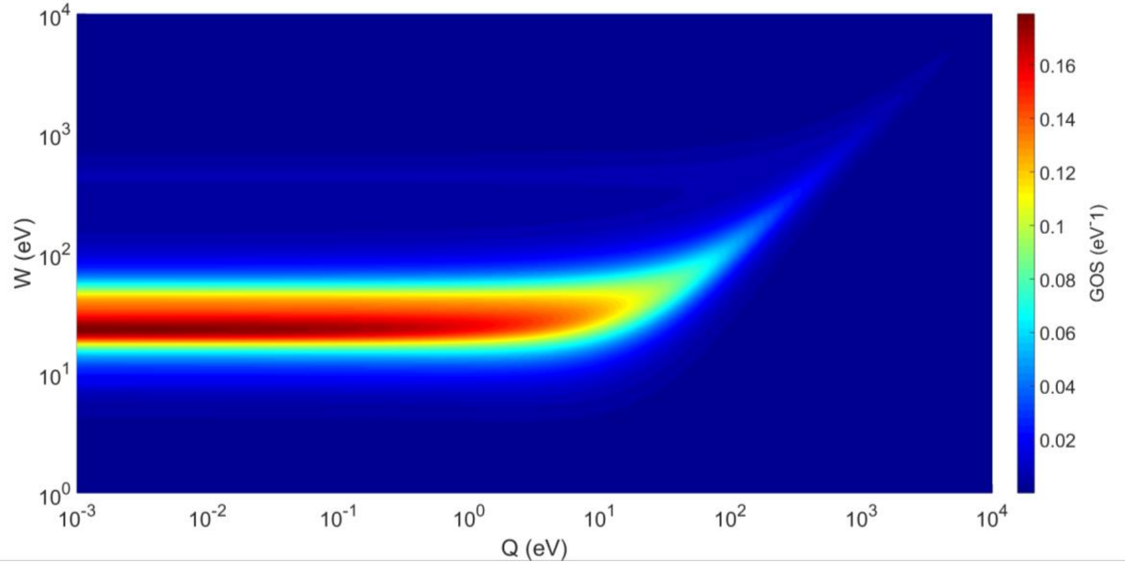
Q=0 → **Q≠0**



Total GOS



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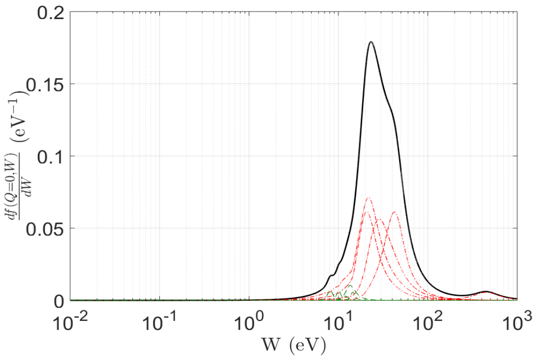

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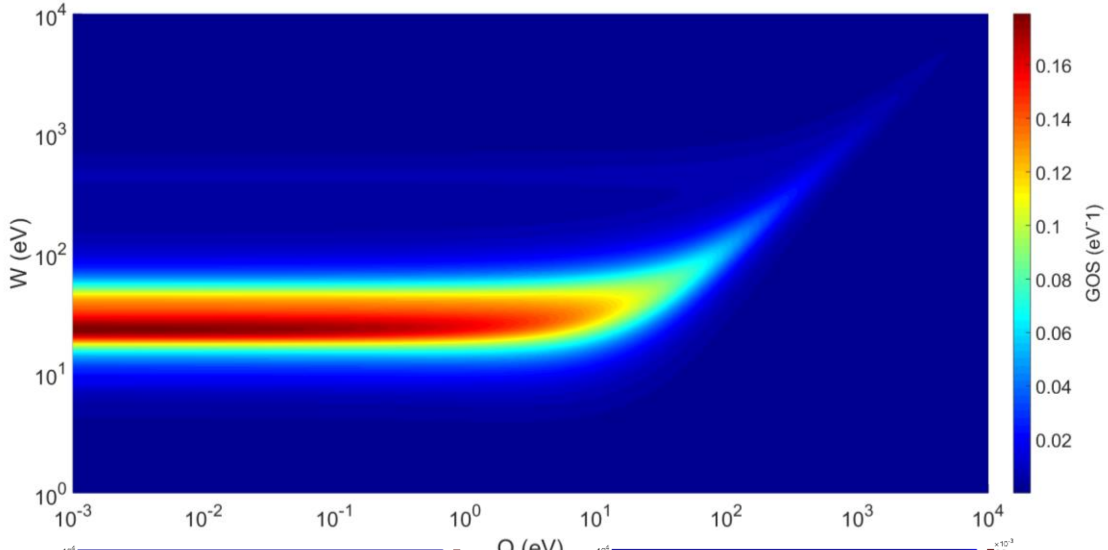
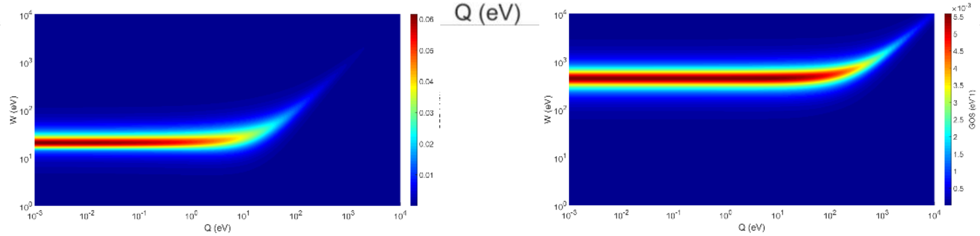


Q-extension is complex

low-Q GOS ≈ constant

Large-Q Bethe Ridge (Q=W)



Shell Ionization GOS

GOS of liquid water

GOS model (asymptotic behavior)

[F. Salvat / *NIMB 316 (2013) 144–159*]

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

- Small Q dominates in transverse interaction
- Differences between GOS and TGOS are negligible at small Q

$$\int_0^\infty \frac{df(Q,W)}{dW} dW = Z_M$$ → Bethe sum rule

$$Z_M \ln I = \int_0^\infty \ln W \cdot \frac{df(Q=0,W)}{dW} dW$$ → I-value definition

The model reproduces Bethe formula for the **stopping power**

Optical-Impulse approximation

$$\frac{df(Q,W)}{dW} = \sum_j F_j \left[\underbrace{p_j(W)\Theta(Q_j - Q)}_{\text{Low-Q (distant)}} + \underbrace{\delta(Q-W)\Theta(Q-Q_j)}_{\text{Large-Q (close)}} \right]$$

Low-Q (distant)

Large-Q (close)

Target electrons react as if they were free and at rest

Results

Differential Cross Section (DCS)

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

No experimental data available for our E values

Comparison with G4-DNA current models

Total Cross Section

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

No experimental data available for our E values

Comparison with oxygen K-shell data from PenH

Stopping Power

$$\mathcal{S} = \mathcal{N} \int_0^E W \frac{d\sigma}{dW} dW$$

Comparison with PSTAR database

Results

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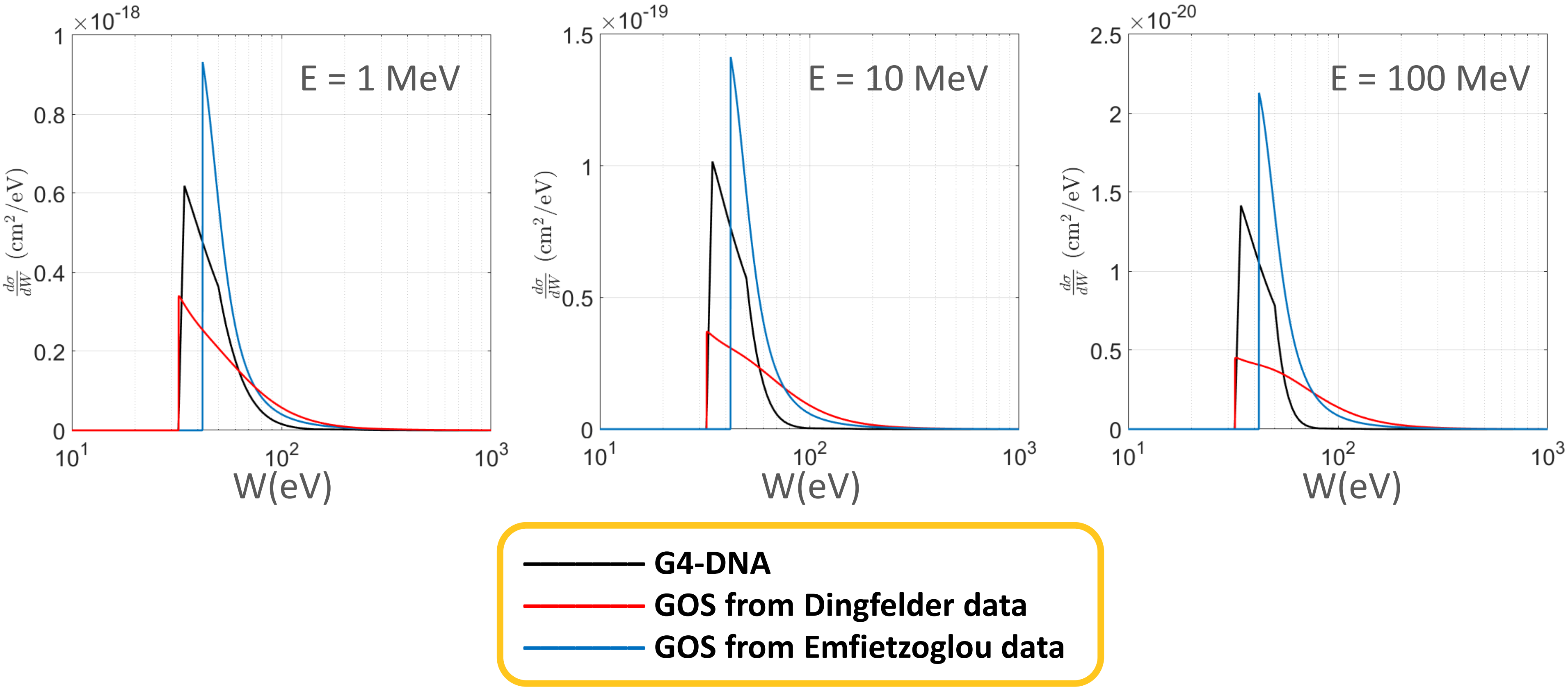

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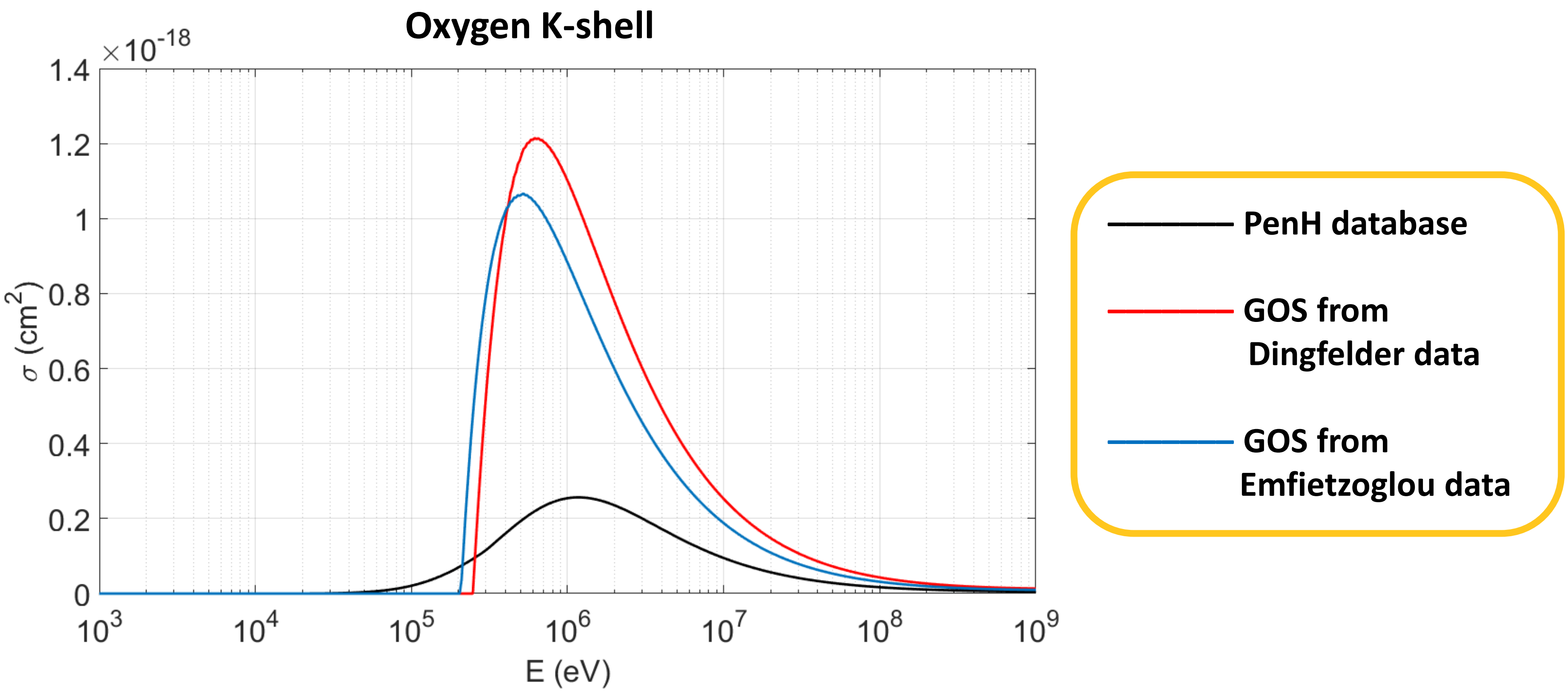

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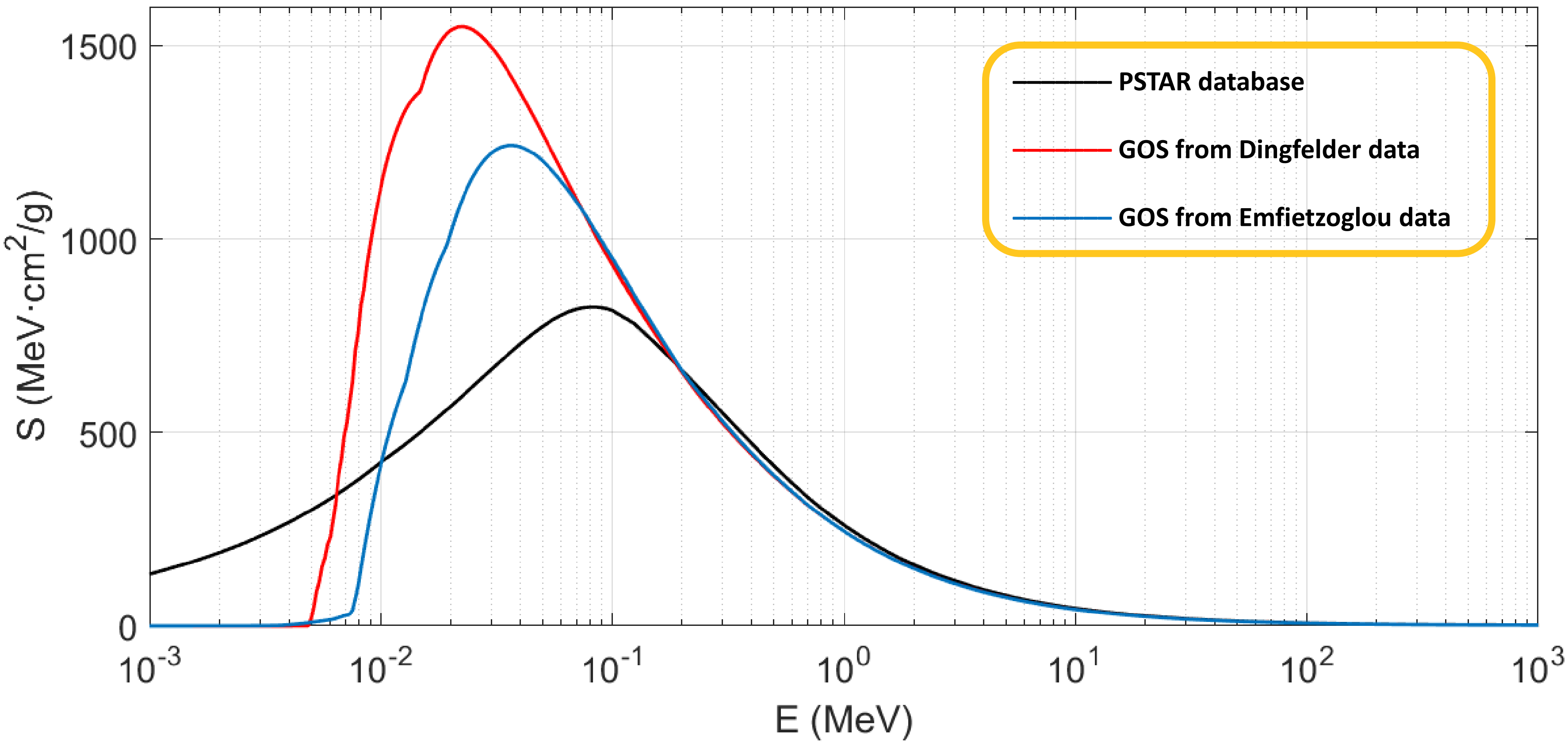

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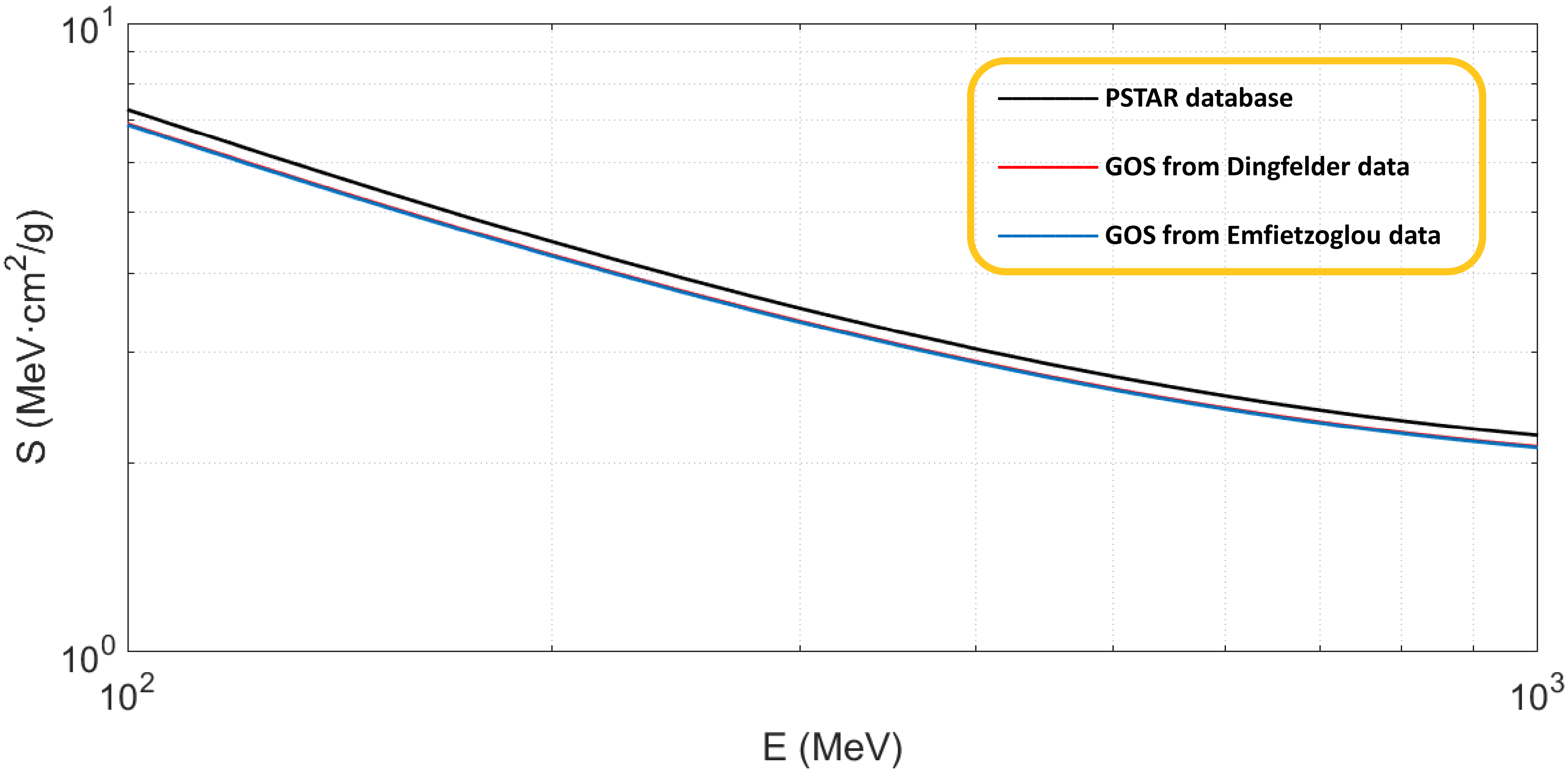

Conclusions and future work

- RPWBA theory offers a start point to calculate differential cross sections.
- GOS characterizes the response of the material.
- Results obtained with an asymptotic GOS model shows a good correspondence with PSTAR stopping power in the range of interest.
- There are no cross section and DCS experimental data for incident energies of the order of 100 MeV. Differences with current G4-DNA data are due to GOS models.
- Next, with more detailed models for GOS we will produce the cross section databases to be included for Geant4-DNA

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