http://geant4-dna.org

Development of a New Geant4-DNA Electron Elastic Scattering Model for Liquid-phase Water Using the ELSEPA Code

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May. 8, 2019 – Jeju, Korea

The results in this presentation were published in:
W.G. Shin et al. (2018) *J. Appl. Phys.* ***124*** *224901.*

Contents

- Background
- Electron elastic scattering modeling
- Influence on track structure simulations
- Influence on radiolysis simulations
- Conclusion

Biological effects induced by ionizing radiation

- In order to understand low-dose radiation carcinogenesis, the evaluation of biological effects induced by ionizing radiation is a major scientific challenge

L. Mullenders et al. (2009) *Nature Reviews Cancer* **9** 596.

- The Monte Carlo method is typically employed to evaluate radiation effectiveness

Monte Carlo method - e.g.) the Geant4 toolkit

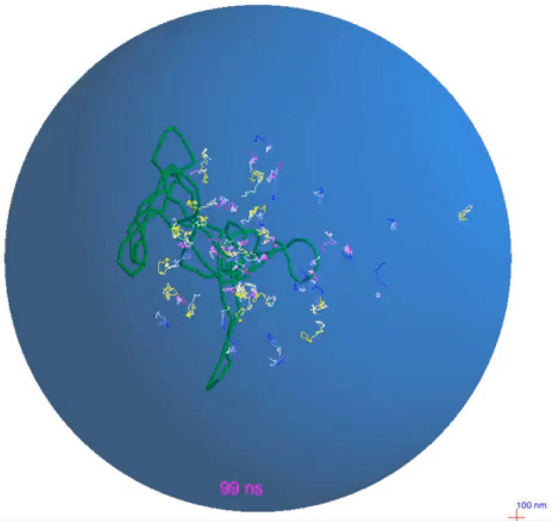
http://geant4.org

- Computational technique based on random number generation
  - Can accurately simulate the stochastic nature of particle-matter interactions
- General purpose Monte Carlo tools have been developed (e.g. Geant4)
  - Open source
  - "expandable" by the user
- However, Geant4 is not suitable to estimate biological damage
  - Condensed-history approach
  - Cannot transport molecules
  - Only physical particle-matter interactions

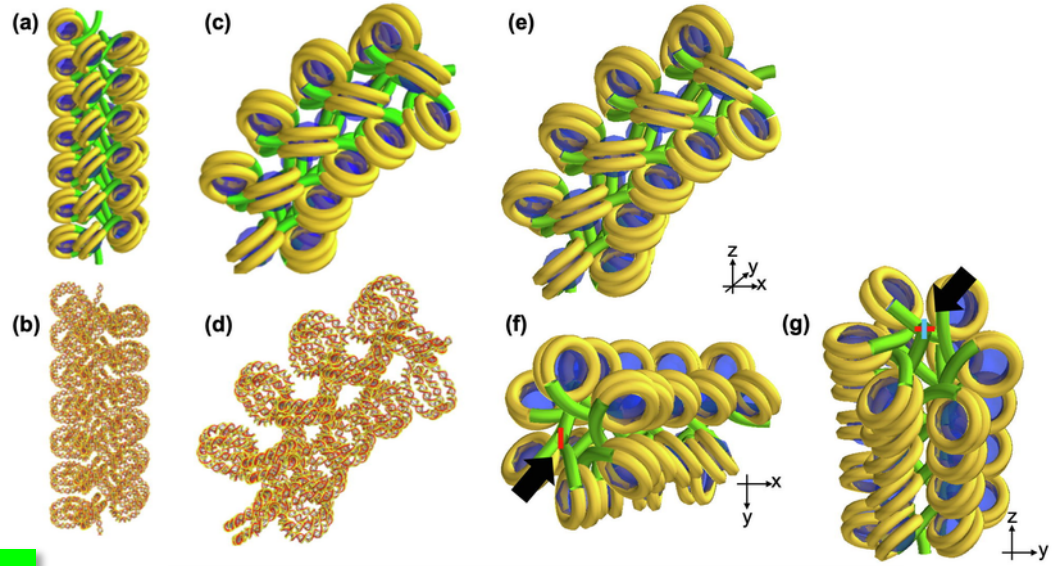
Monte Carlo track structure simulation - e.g.) Geant4-DNA

http://geant4-dna.org

- The Track Structure (TS) Monte Carlo method is today the most reliable approach to evaluate biological effects induced by ionizing radiation
  - Step-by-step transport of physical particles (e.g. electrons)
  - Molecular species simulation (e.g. hydroxyl radicals)
  - Target properties (e.g. molecular cross sections, biological geometry)



Irradiation of a pBR322 plasmid, including radiolysis
- movie courtesy of V. Stepan
(NPI-ASCR/CENBG/CNRS/IN2P3/ESA)



Segments of human chromatin
D. Sakata et al. (2019) *Phys. Med*. In press

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http://geant4-dna.org

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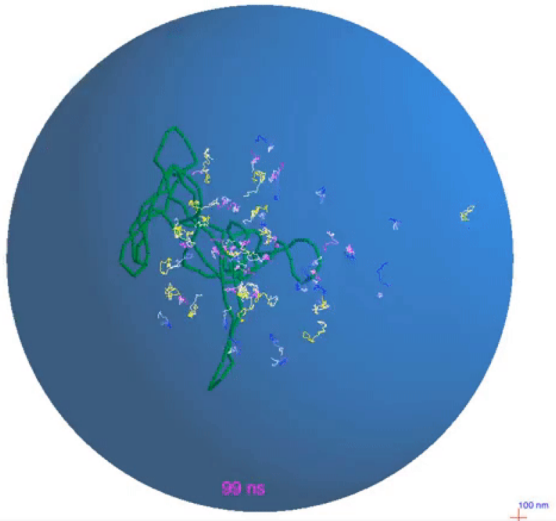

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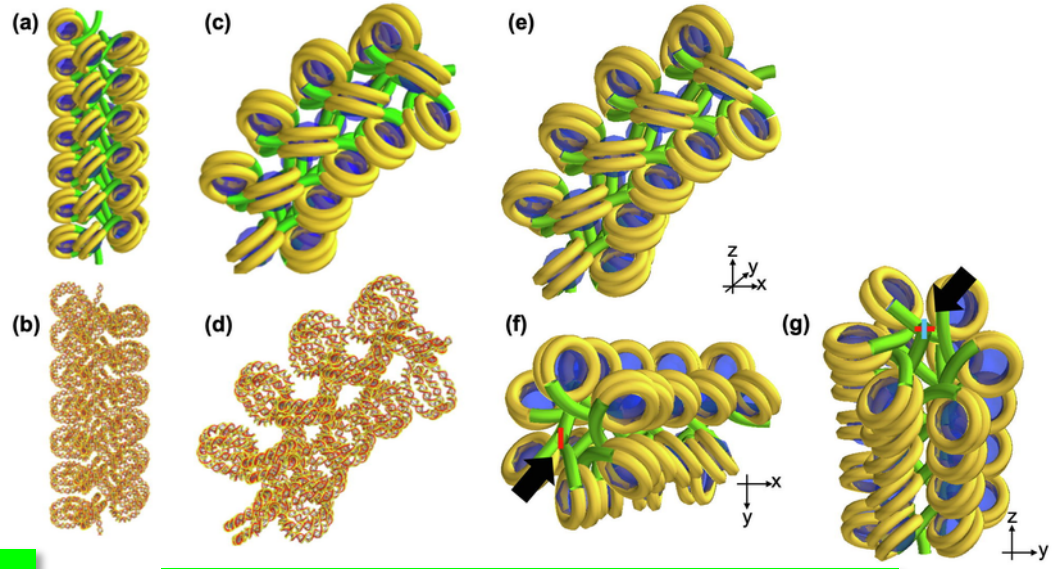

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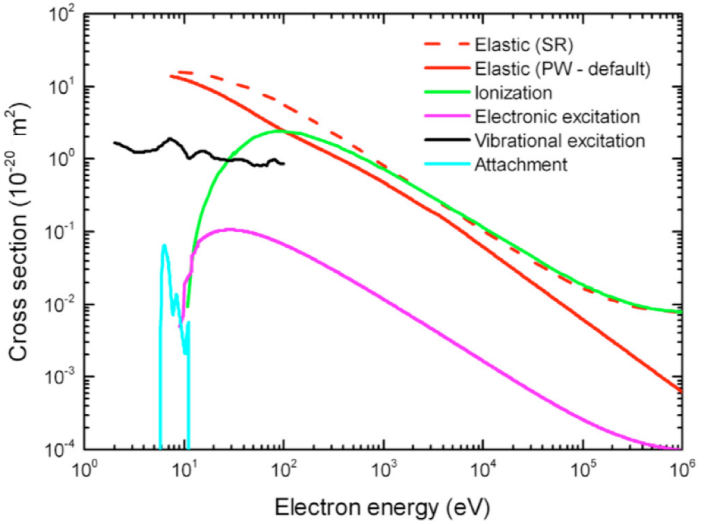
Step-by-step transportation

- To accurately simulate step-by-step particle transportation, accurate cross sections are needed

- In particular, low energy secondary electrons are important for the study of radiation damage to DNA in the cell nucleus
  - Inelastic interactions induce direct damage
  - Elastic interactions determine electron "concentration"

Elastic scattering in liquid water

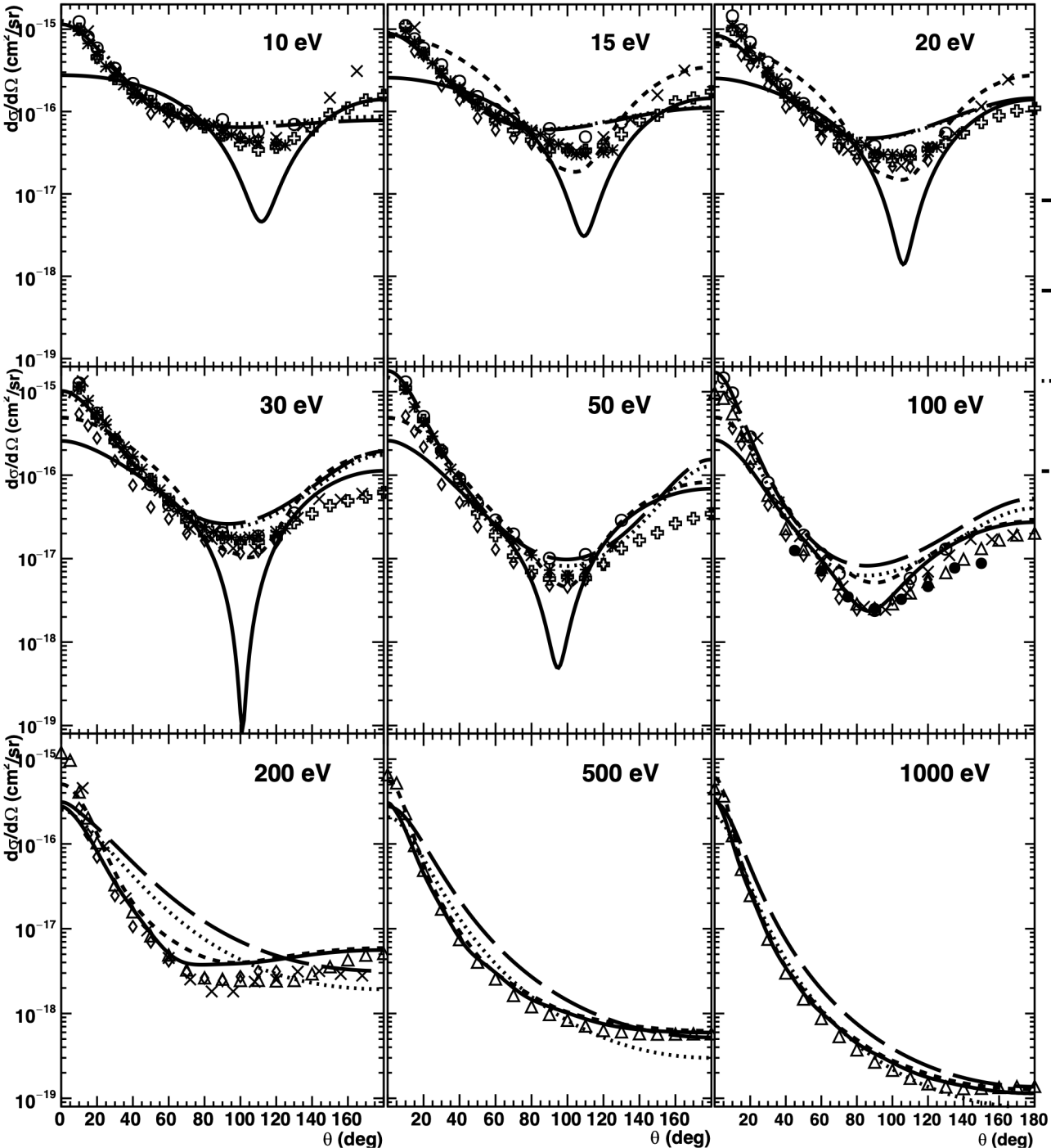
- At low energy (< 100 eV), elastic scattering plays a key role
  - Even if elastic scattering is not associated with significant energy loss, it allows to describe the spatial distribution of electrons



S. Incerti et al. (2014) *Nucl. Instrum. Meth. B* **333** 92.

- We propose to improve the accuracy of the modelling of electron elastic scattering in liquid water
  - To be used in particular in combination with soa inelastic models developed at Ioannina U., in Greece

Elastic scattering angular Differential Cross Section (DCS)



In Geant4-DNA

- Partial wave
- Screened Rutherford
- Uehara Screened Rutherford
- CPA100

- Hilgner et al. (1969)
- Danjo and Nishimura (1985)
- Johnstone and Newell (1991)
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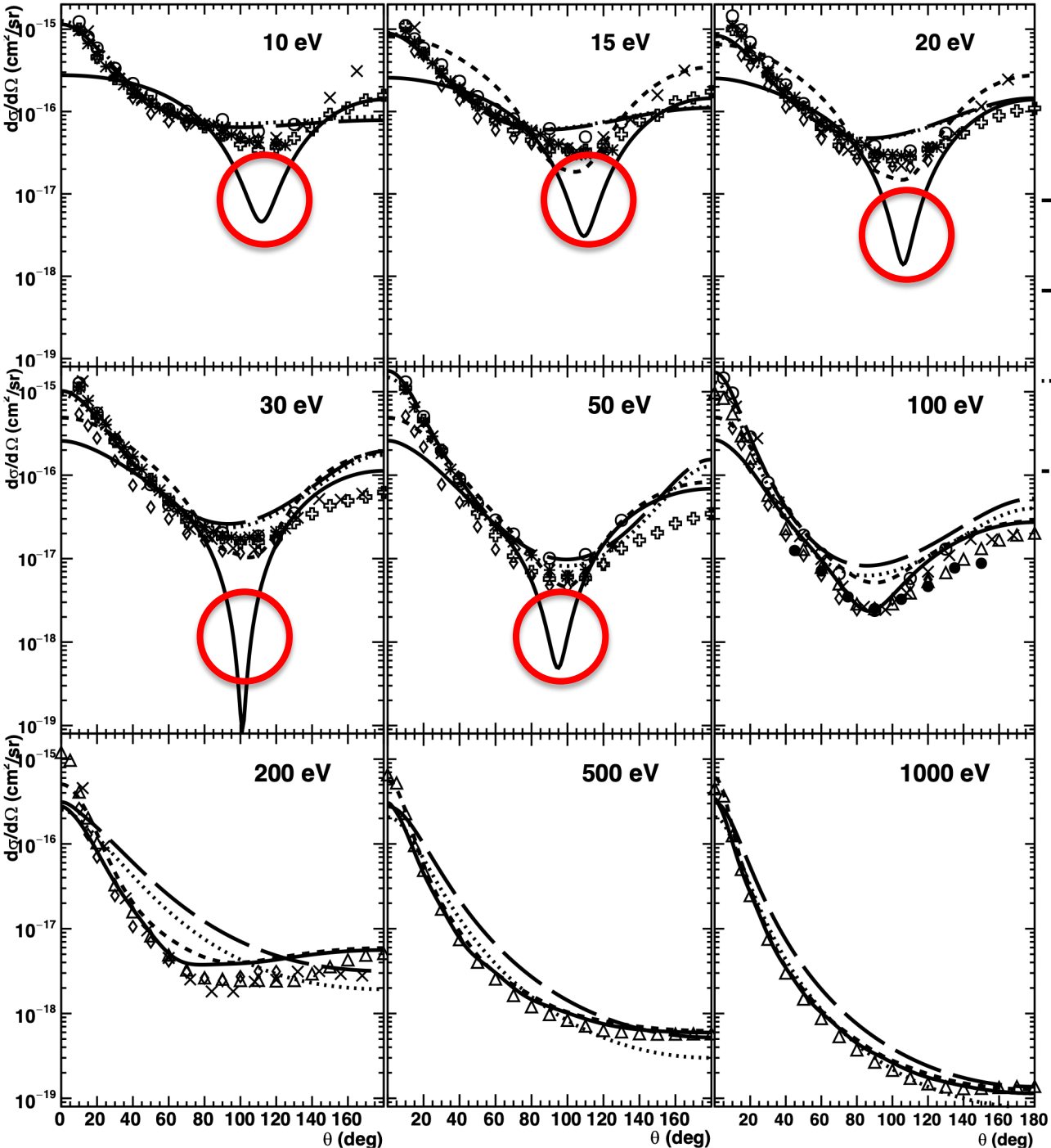

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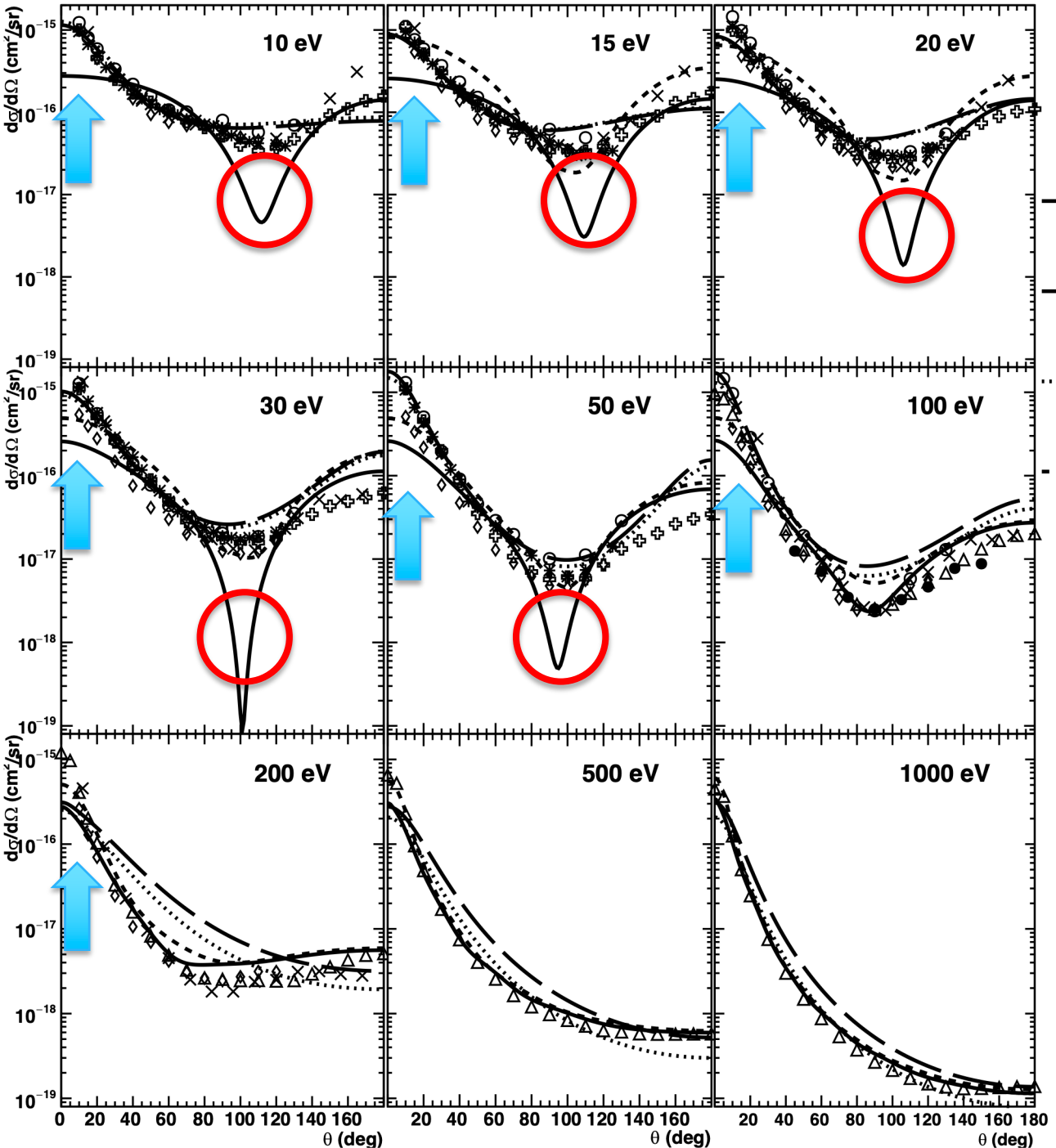

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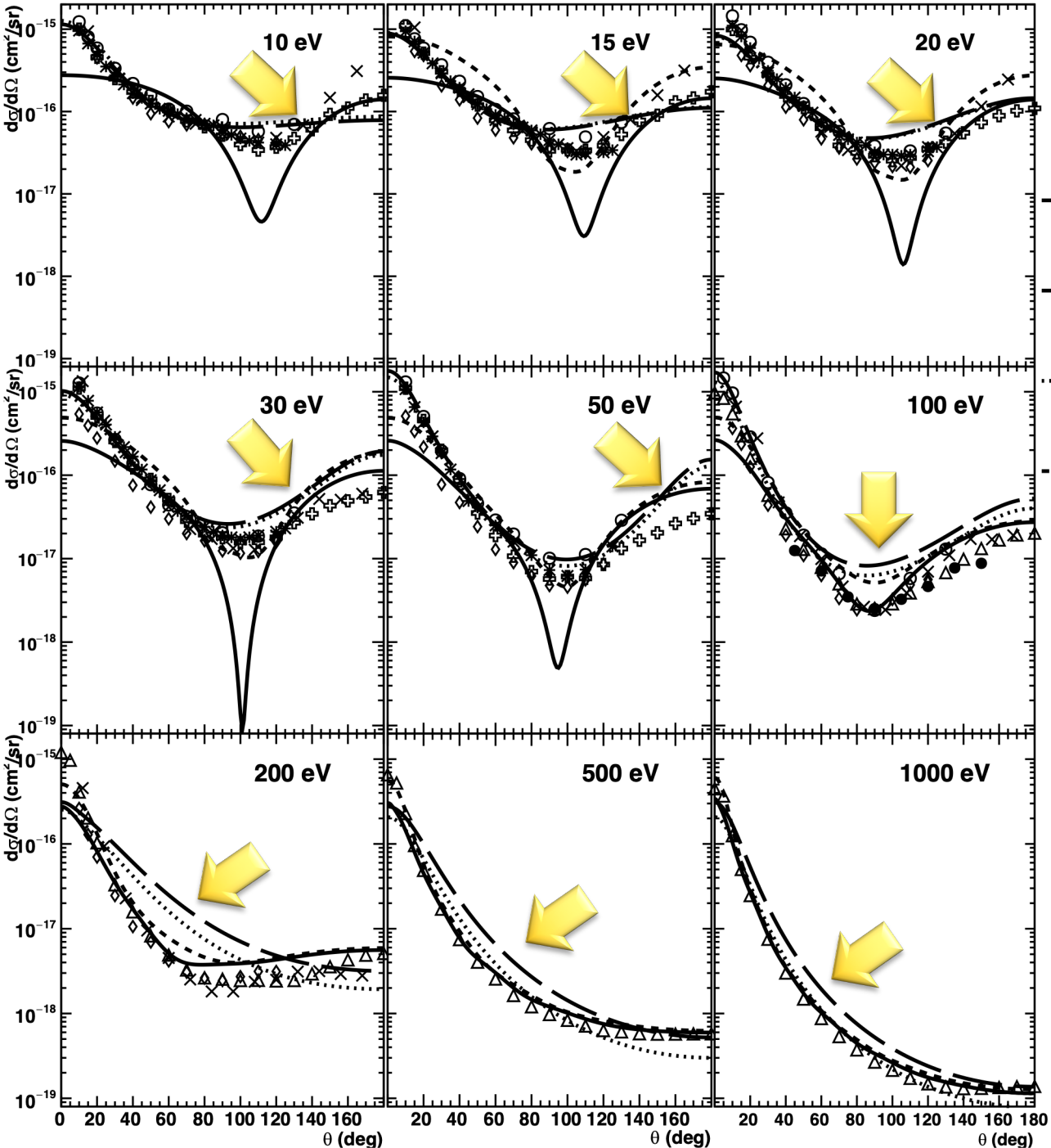

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Improving elastic scattering

- The purpose of this study is to develop a new electron discrete elastic scattering model for Geant4-DNA using the ELSEPA code developed by *Salvat F. et al.* (Barcelona U.)
  - Unfortunately ELSEPA can not handle liquid phase of water

F. Salvat et al. (2005) *Comput. Phys. Commun.* **165** 157.

- Steps
  1. We first optimize the phenomenological parameters of ELSEPA, using experimental data in the vapour phase water, assuming the free atom approximation
  2. We then try to calculate the elastic cross section in liquid water using the Muffin-tin approximation, typically employed to predict interaction in solid phase material

- In order to evaluate the impact of this new model on TS simulations, we performed range, dose-point-kernel, and water radiolysis simulations and compared to existing models available in Geant4-DNA

1) Optimization of ELSEPA parameters using vapour data

$$V(r) = V_{st}(r) + V_{ex}(r) + V_{cp}(r) - iW_{abs}(r)$$

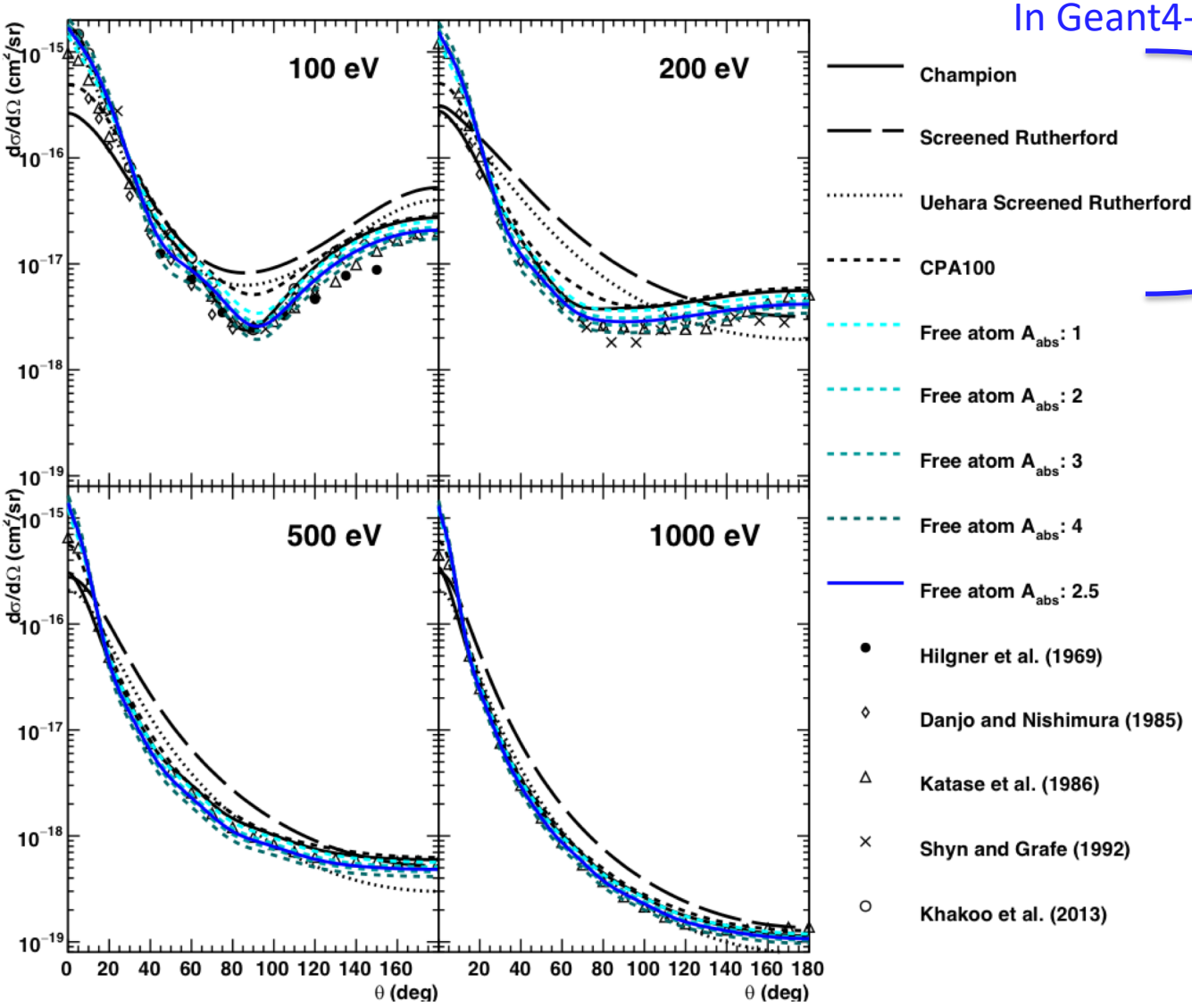
- Correlation-polarization potential for long-range trajectories V_{cp}
  - Buckingham as default
    - Lindhard model as an alternative option for Muffin-tin approximation
  - Influences small scattering angle

- Adjustable energy dependency b_{pol} for V_{cp}
  - $b_{pol} = \sqrt{\max\{(E - 50)/16.1\}}$ as default
  - Influences small scattering angle

- Absorption strength A_{abs} for inelastic absorption potential W_{abs}
  - For water, ICRU-77 report recommends a value of 2
  - Influences intermediate and large scattering angle

- As an example…

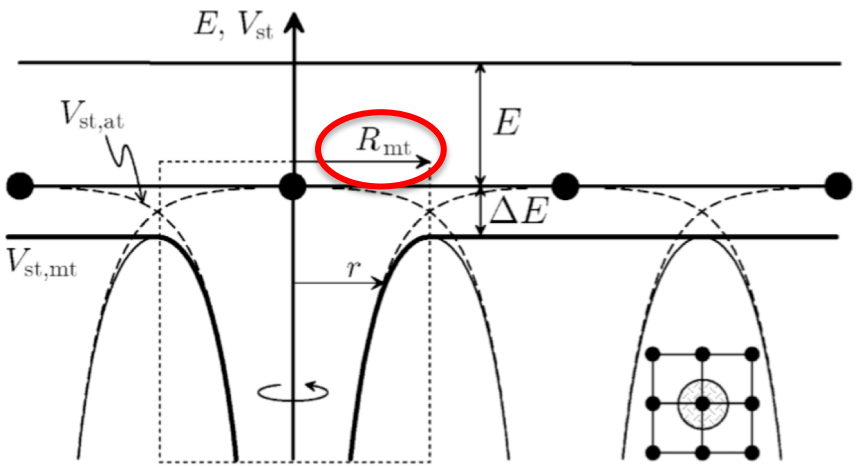
Example of optimization: A_{abs}



In Geant4-DNA

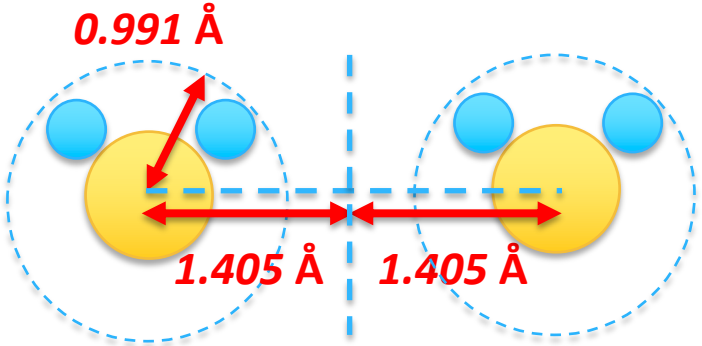
- DCSs are calculated according to the proposed parameters
- The results are compared with experimental data based on the DCS values at 0 deg and on RMSE
- The optimal values are then selected

2) Muffin-tin approximation



D. Bote et al. (2009) *J. Electron Spectrosc.* **175** 41.

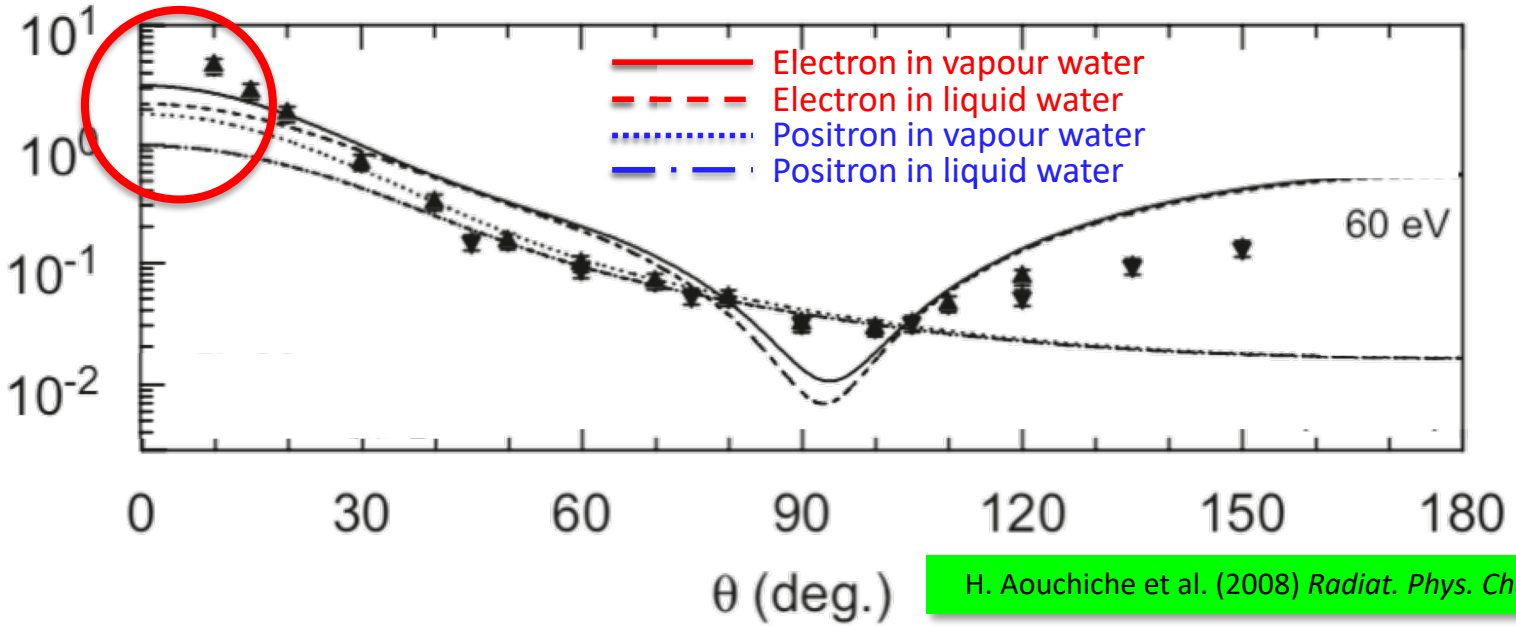
$$\rho_{e,mt}(r) = \begin{cases} \rho_e(r) + \rho_e(2R_{mt} - r) + \rho_u, & r < R_{mt}, \\ 0, & r > R_{mt}, \end{cases}$$



- The atomic electrons are assumed to be confined within a sphere of finite radius, R_{mt}
- This approximation is typically employed to predict cross sections in solid-phase material
- Muffin-tin radius selected: 1.405 Å.
  - Half distance between oxygen atoms in liquid water

D. Liljequist et al. (2012) *Int. J. Radiat. Biol.* **88** 29.

Verifying the plausibility of calculations using exp. data in vapour water



H. Aouchiche et al. (2008) *Radiat. Phys. Chem.* **77** 107.

- Unfortunately, no data exists in the liquid phase, so there is no way to fully validate cross sections for the liquid phase
- Calculations based on a partial-wave formalism with a Dynamic Molecular framework have been proposed by Aouchiche et al. (2008)
  - The DCSs for liquid water are slightly lower (~ 2/3) than the DCSs for vapor water at 0°
- Taking into account such expected differences, we can check our ELSEPA calculations
  - DCSs for liquid should be generally smaller than for the vapour phase at small scattering angle

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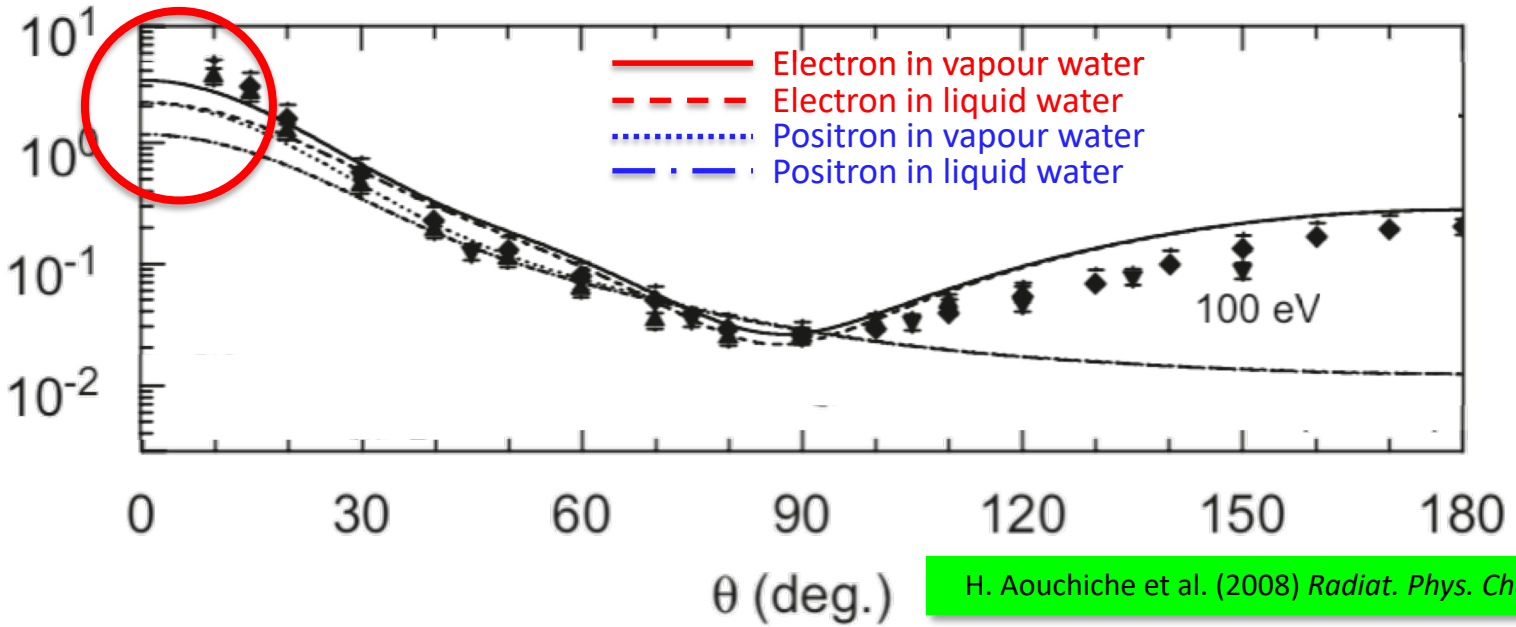

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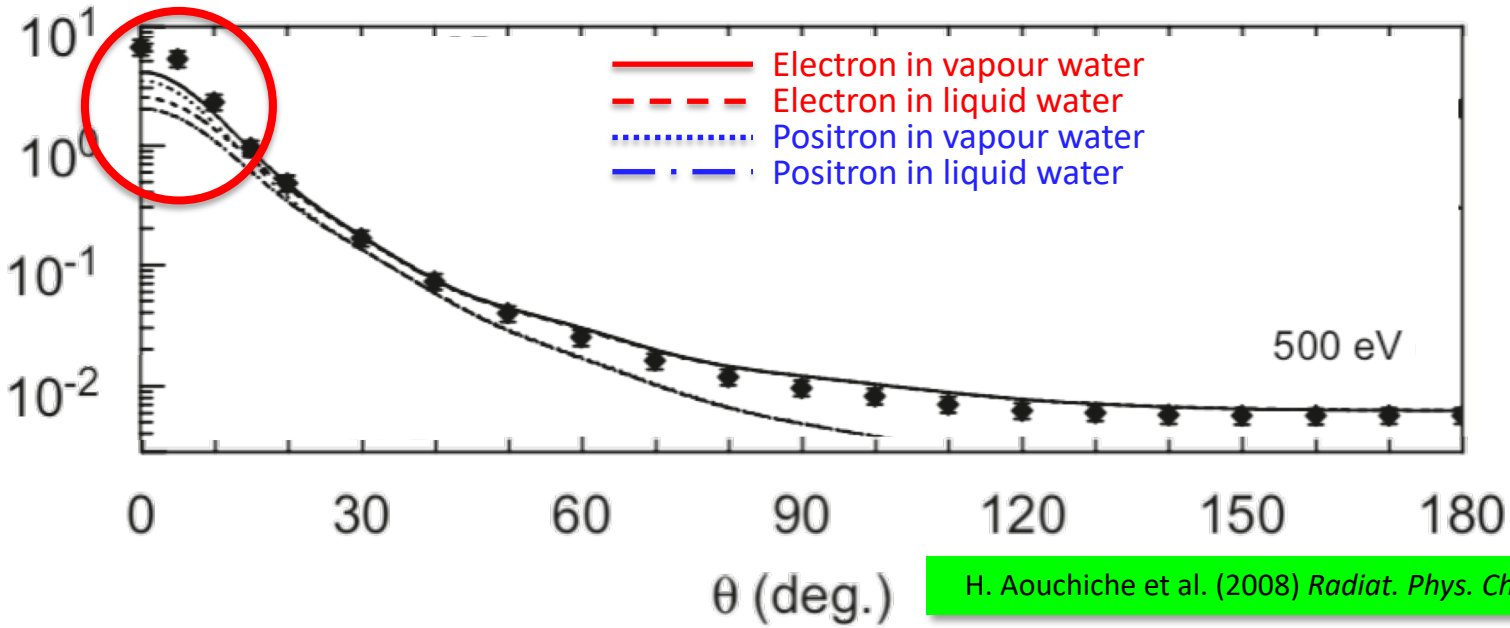

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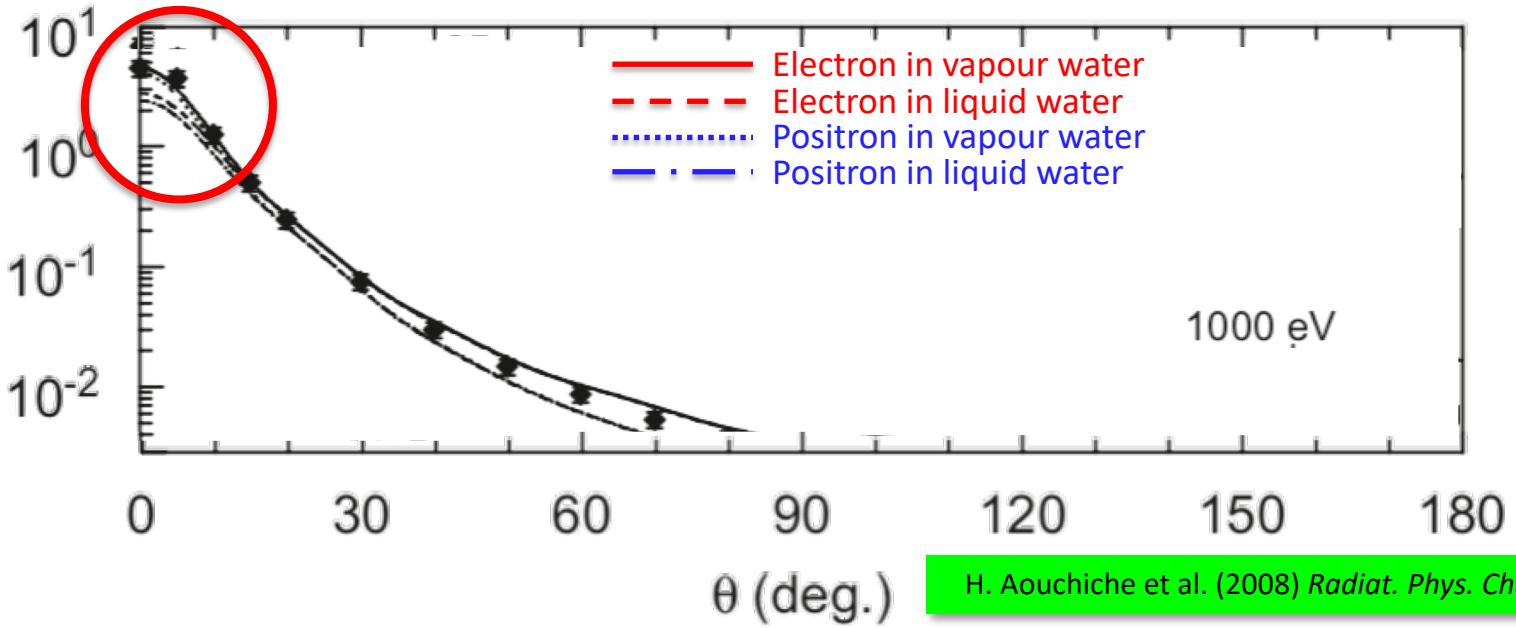

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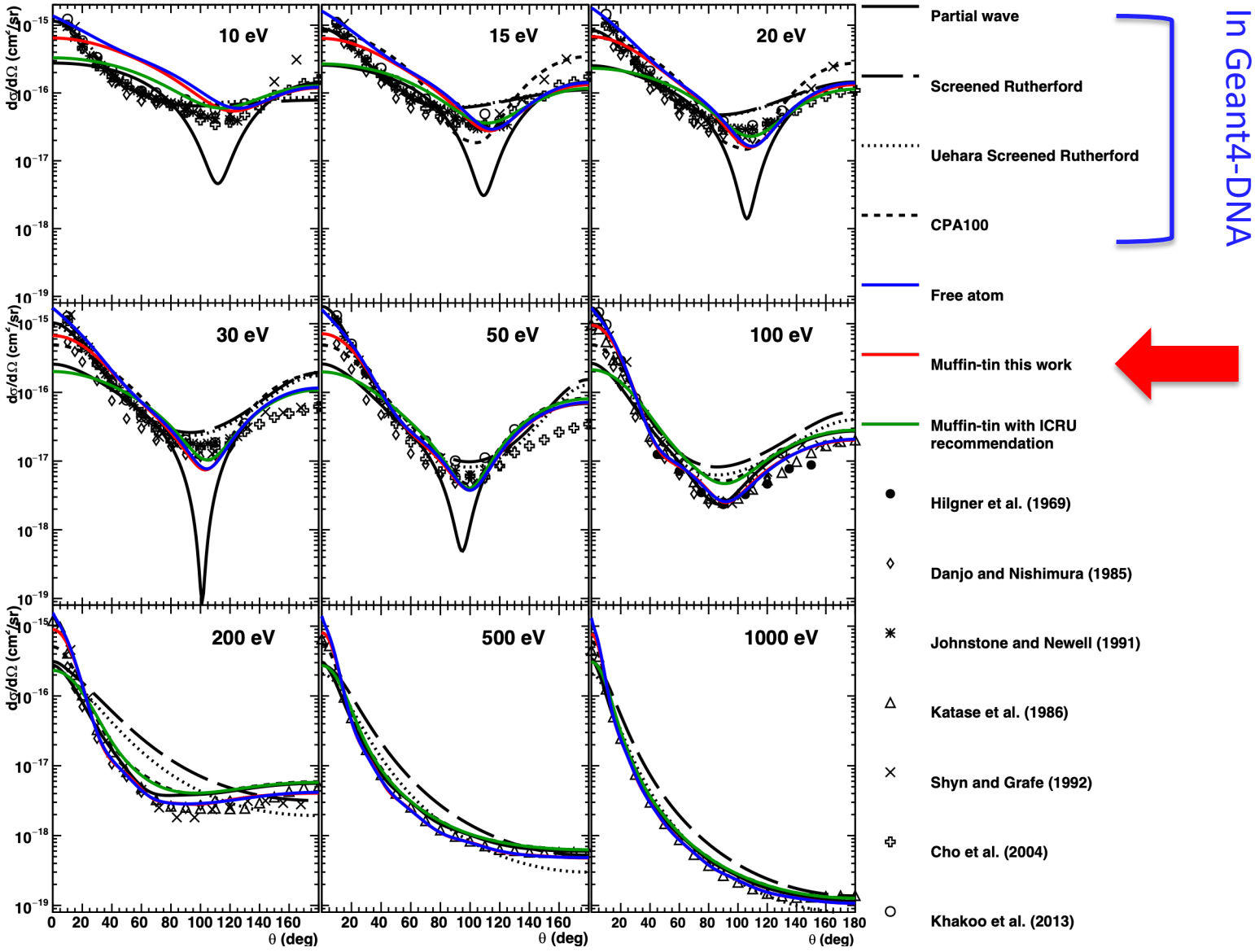
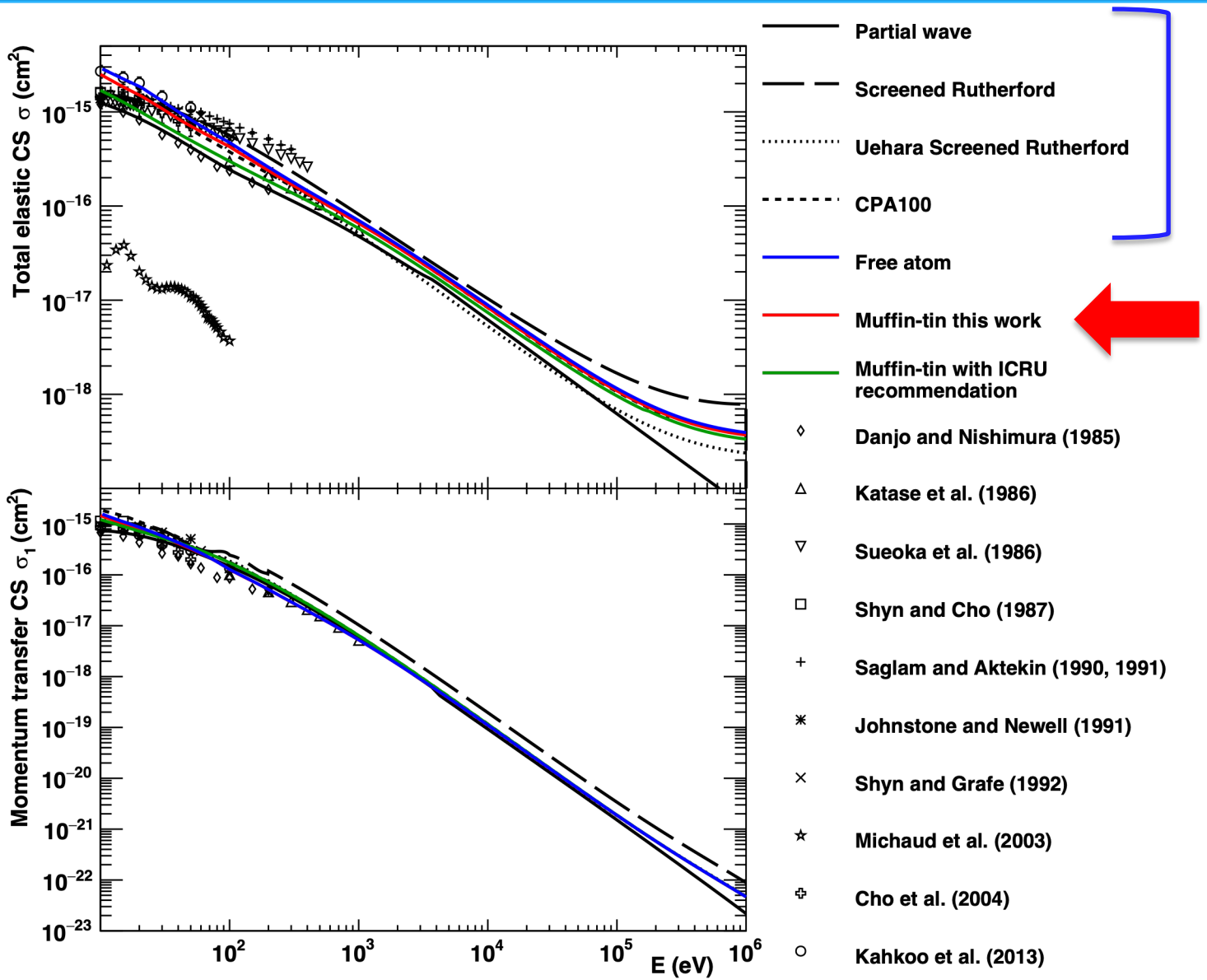
Results (1): Differential Cross Section (DCS)



Results (2): Total Elastic Cross Section (TECS) and Momentum Transfer Cross Section (MTCS)



Track structure simulations - Geant4-DNA examples

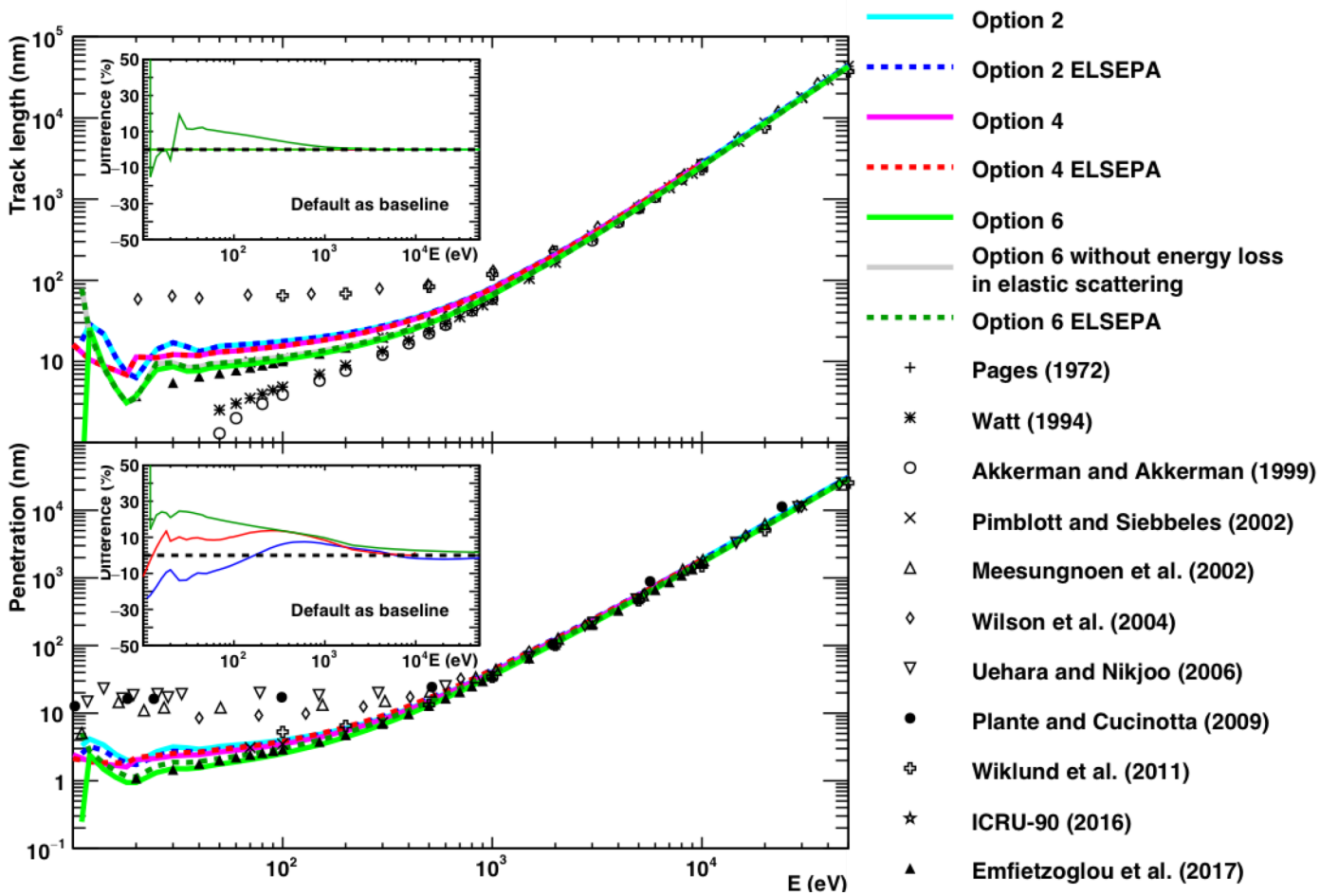
Three examples

- range example
  - Accumulated "Track length (nm)"
  - Distance between initial and final position, "Penetration (nm)"
- TestEm12 example
  - Energy deposition as a function of the distance from the source, "Dose-point kernel (nm/eV)"
- chem6 example (new: created for this work)
  - The number of molecular species "G value (#/100 eV)"
    - G values versus time
    - G values versus linear energy transfer (LET)

And six Geant4-DNA Physics constructors for electrons

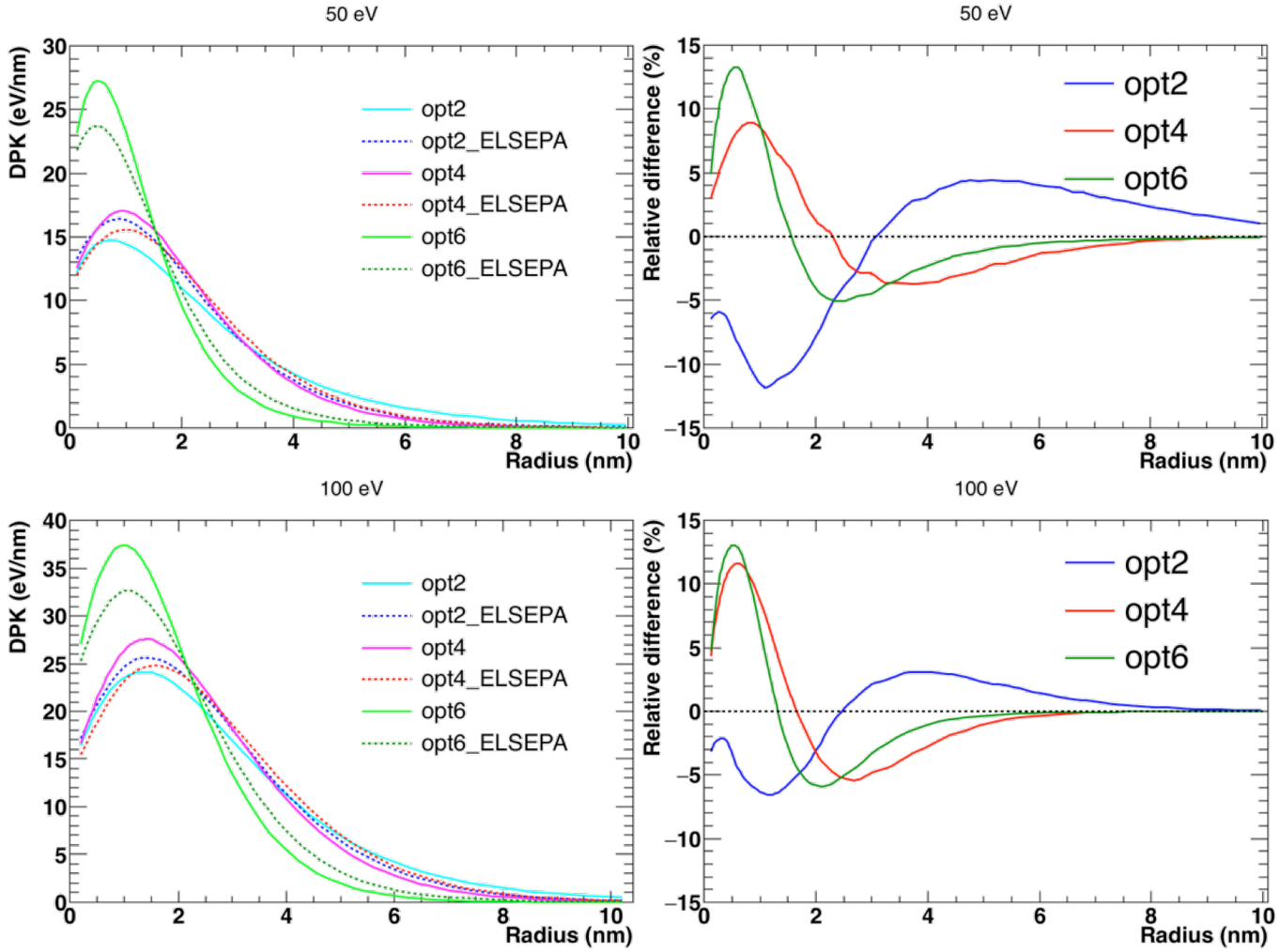
- Option2, 4, and 6 with and without new ELSEPA based elastic model

Track length and penetration



- Elastic scattering model doesn't impact track length
  - except for option 6 considering small energy loss in elastic scattering (based on CPA100 MC code)
- Less elastic scatterings and smaller scattering angles induce longer penetrations
- The relative differences are less than 20% at low energy

Dose-Point Kernel (DPK) @ 50 and 100 eV

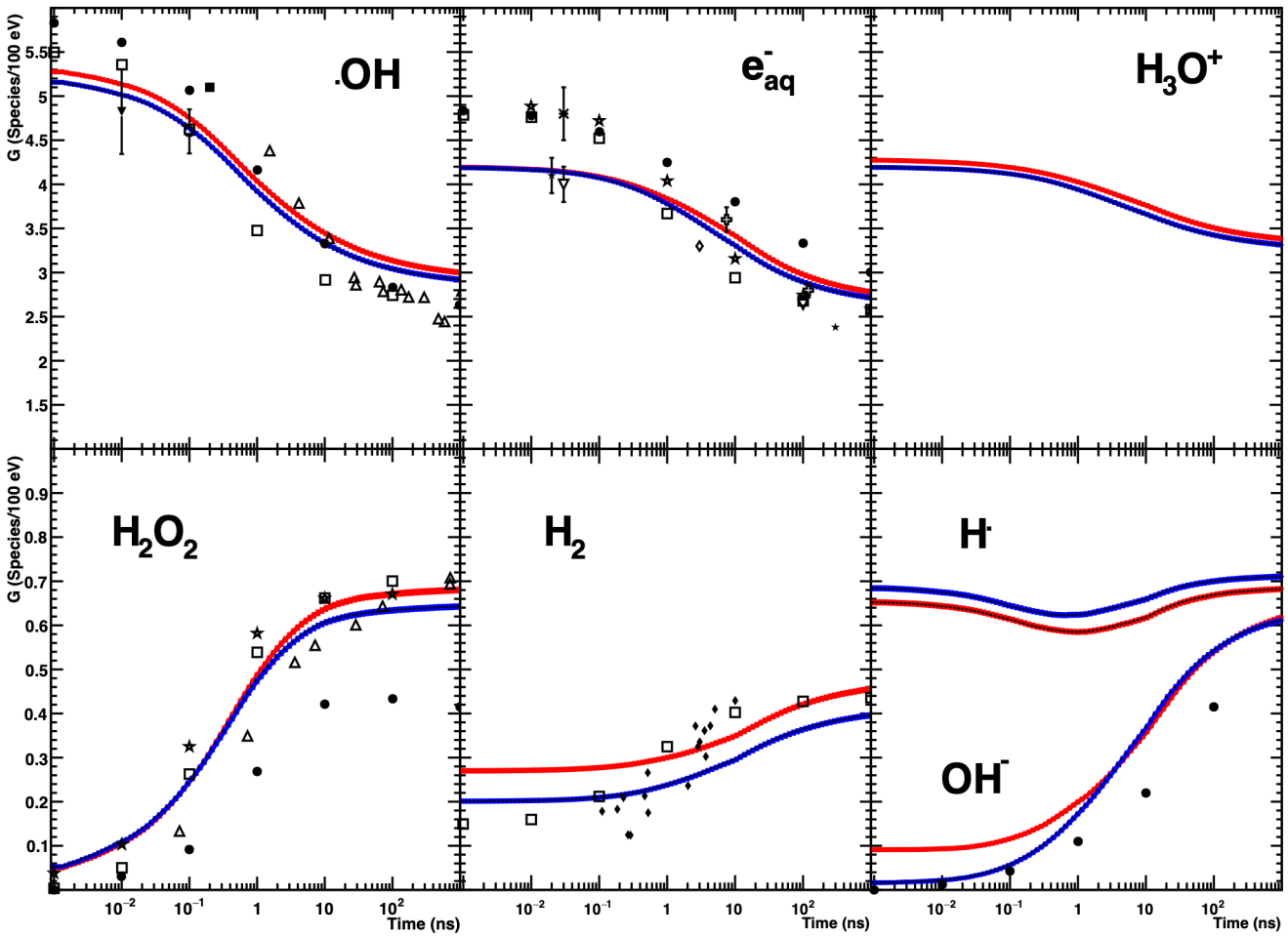


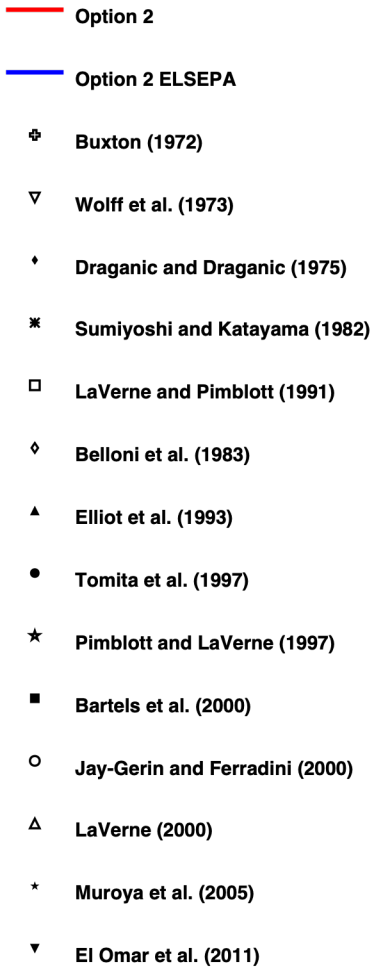
- Relative difference based on the equation:
  - $\Delta(r) = \frac{\delta E_{EL}(r) - \delta E_{def}(r)}{\max(\delta E_{EL}, \delta E_{def})} \times 100\ (\%)$

Maigne et al. (2011) *Phys. Med. Biol.* **56** 811.

- Option 2 is more diffusive than option 2 ELSEPA at low energy, which is not the case for the two other options
- These results have direct influence on electron concentration

Water radiolysis results - G versus time





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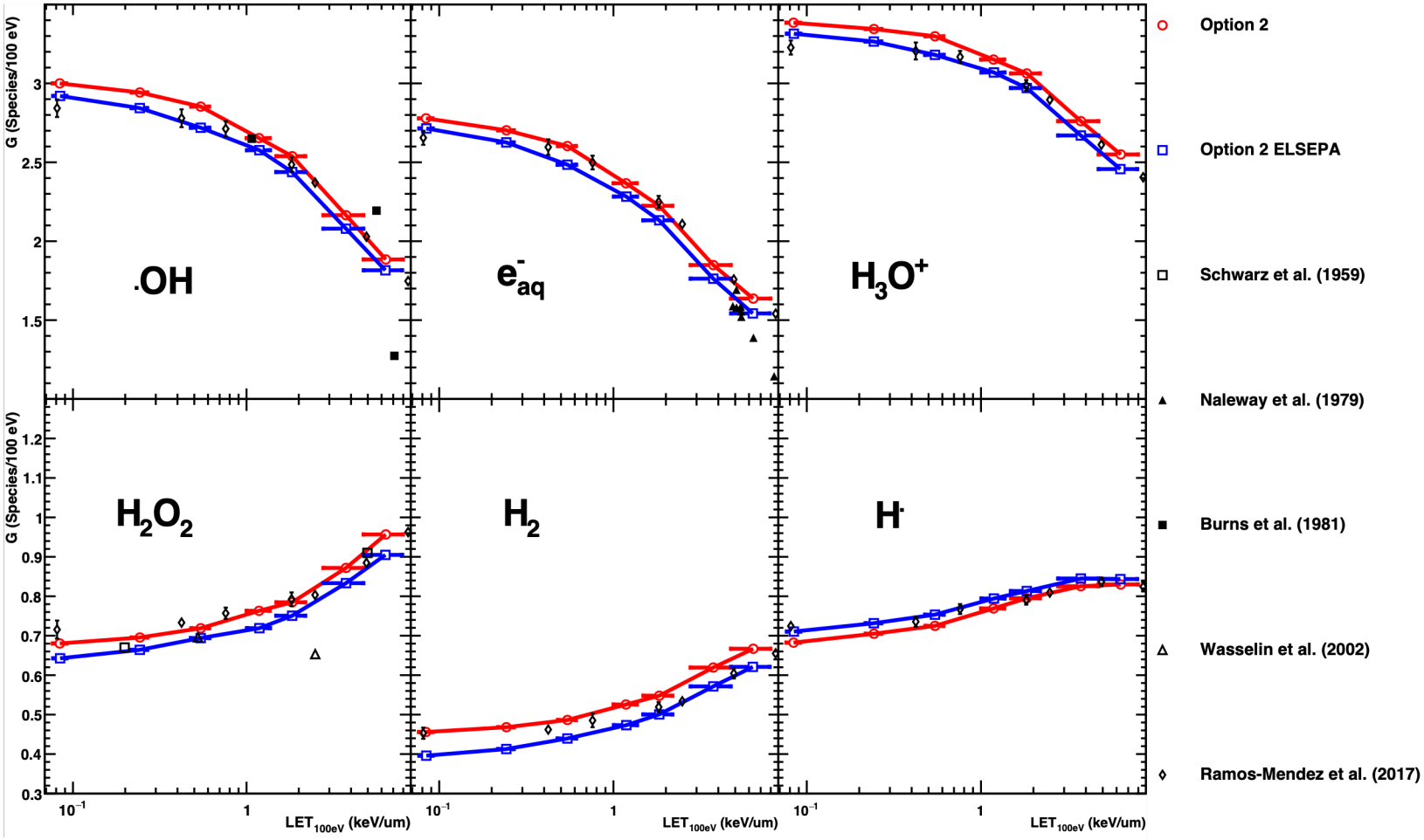
W.G. Shin et al. (2019) *J. Appl. Phys.* Under review

Water radiolysis results - G versus LET



W.G. Shin et al. (2019) *J. Appl. Phys.* Under review

Conclusions

- We propose a new electron elastic cross section model for liquid water based on ELSEPA assuming the Muffin-tin approximation
- The phenomenological parameters including correlation-polarizability potential and inelastic absorption potential have been qualitatively optimized
- The DCSs show improvement versus the other existing Geant4-DNA models such as the SR, USR, and partial wave models, comparing to experimental data
- The simulations with the new elastic model show reasonably good agreement with all physics constructors in Geant4-DNA
  - Up to about 20% at low energy for range and DPK
  - Up to about 6% for water radiolysis simulations for option 2
- This model will soon be released in Geant4

Thank you very much for your attention !