"G4DNA" low energy physics processes for protons and electrons in liquid water

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Plan

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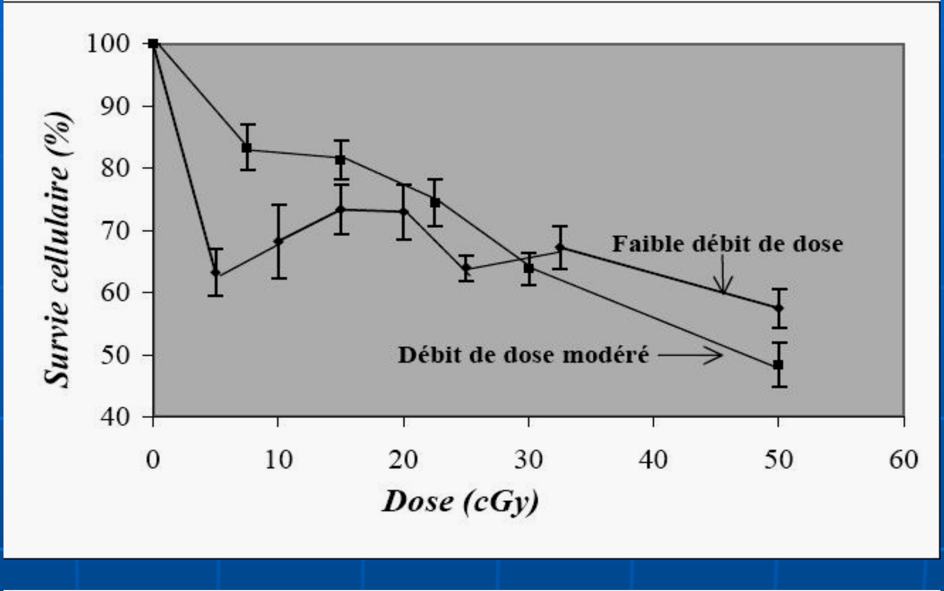
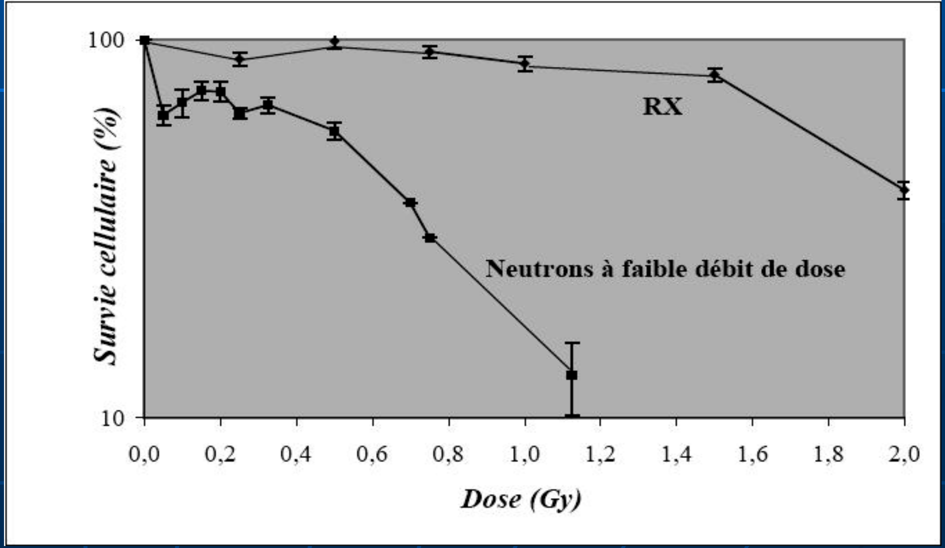
1- Introduction

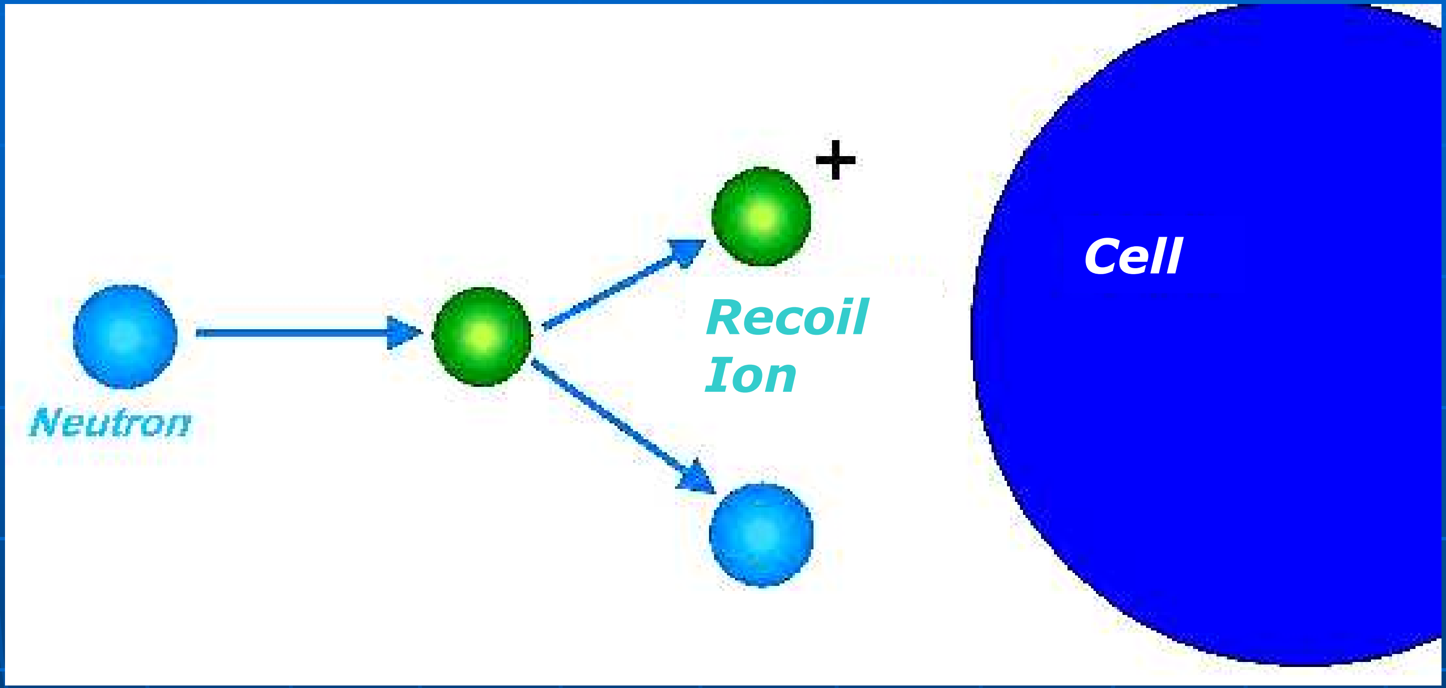
- With our neutron irradiation facility at LPC Clermont-Ferrand we can irradiate human cells with 14 MeV neutrons at 5cGy/h dose rate.
- Cell survival curves are then obtained for normal cells as well as for melanoma cells and glioma cells.
- In order to understand the cell behavior after irradiation one should be able to estimate the amount of energy deposed in the cell or also in the cell nucleus. Monte Carlo Simulations can play a useful role in this case.
- The needed processes for protons and electrons were implemented in Geant4 in the Geant4-DNA framework.

Cell irradiations



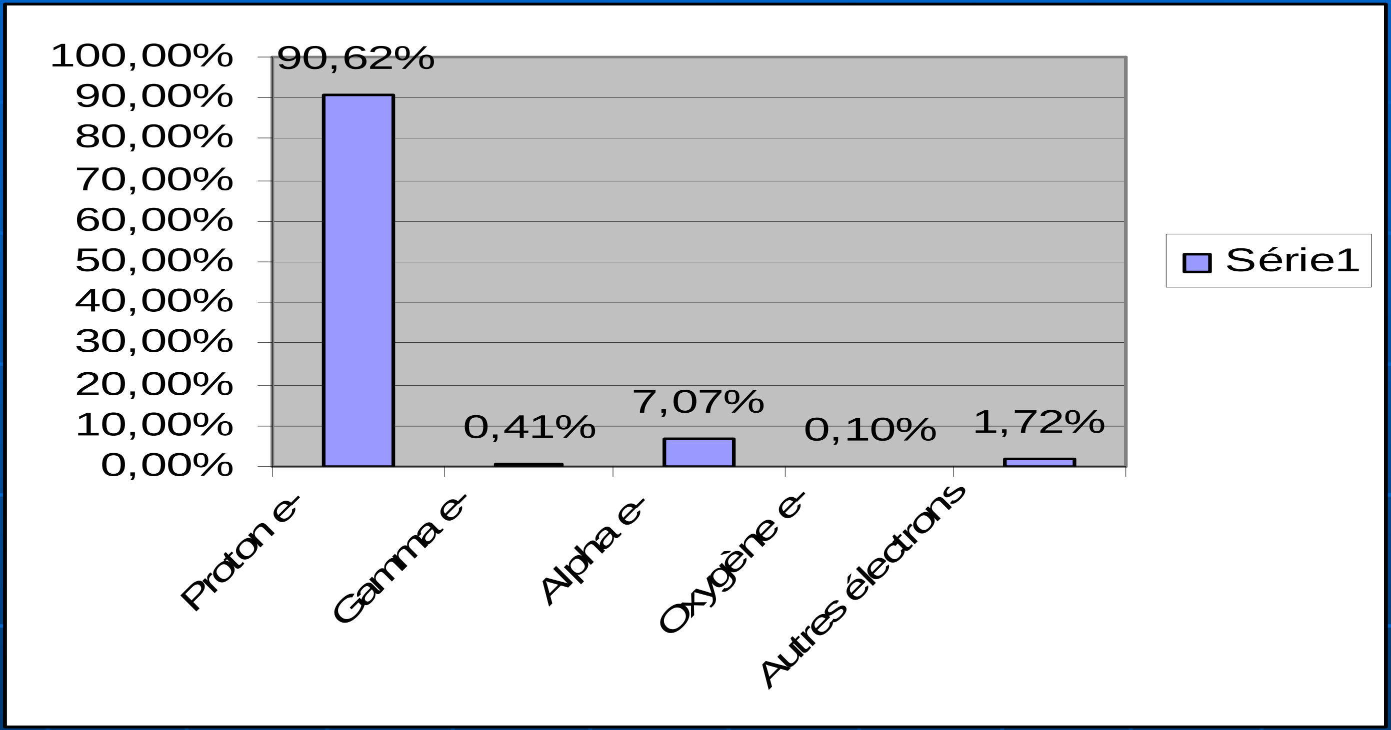


2-Using the Monte Carlo Simulation



- The recoil ions are responsible of delta electrons production.
- The produced electrons can depose energy in the cell, and cause cell (or DNA) damage.

Electron production in water



Percentage of produced electrons in water, shows that almost 90% of electrons are produced by recoil protons.

3- Inelastic interactions in water

An incident proton can lose energy by :

$P + H_2O \longrightarrow P + H_2O^{+} + e-$ **Ionization**

$P + H_2O \longrightarrow P + H_2O^{*}$ **Excitation**

$P + H_2O \longrightarrow H + H_2O^{+}$ **Charge transfer**

$H + H_2O \longrightarrow P + H_2O + e-$ **Stripping**

And electrons can lose energy by :

$e- + H_2O \longrightarrow e- + H_2O^{+} + e-$ **Ionization**

$e- + H_2O \longrightarrow e- + H_2O^{*}$ **Excitation**

Implemented physics processes

Fast Protons (>300keV)	**Ionizations And Excitations**	***Born*** **theory**	***M.Dingfelder, Rad. Phys. and Chem. 59 (2000) 255-275***
Slow Protons (<300keV)	**Ionizations**	***Rudd*** **semi empirical model**	***Rudd, Nucl. Tracks Rad. Meas. Vol 16 no 2-3 p213-218 (1989)***
	Excitations	***Miller & Green*** **semi empirical model**	***Miller & Green, Rad. Reas. 54 343-363 (1973)***
	Charge transfer	***Dingfelder*** **semi empirical model**	***M.Dingfelder, Rad. Phys. and Chem. 59 (2000) 255-275***

Hydrogen	**Ionizations**	***Rudd* semi empirical model (Corrected with scaling factor)**	***M.Dingfelder, Rad. Phys. and Chem. 59 (2000) 255-275***
	Stripping	***Miller & Green* semi empirical model**	***Miller & Green, Rad. Reas. 54 343-363 (1973)***
Electrons	**Ionizations**	***Born* theory**	***D.Emfietzoglou, NIMB B 193 (2002) 71-78***
	Excitations	**•*Born* theory** **•*Emfietzoglou's* semi empirical model**	***•D.Emfietzoglou, NIMB B 193 (2002) 71-78*** ***•D.Emfietzoglou, Phys.Med.Biol. 48 (2003)2355-2371***
	Elastic Collisions	**•Rutherford model (E>200 eV)** **•Brenner model (E<200eV)**	***•D.Emfietzoglou, Phys Med Biol 45 (2000) 3171-3194*** ***•D J Brenner Phys Med Biol (1983) 29 443-447***

4- The *Born* theory

The doubly differential cross section for inelastic collisions is given by the following expression :

$$\frac{d^2\Sigma}{dE\,.dK} = \frac{1}{\pi\,.a_0\,.T}\,\frac{1}{K}\,\eta_2(E,K)$$

$T = \frac{m_{e-}}{M}\tau$ τ is the kinetic energy of the incident particle

E represents the transferred energy during the collision.

K represents the transferred momentum during the collision.

η_2 is the dielectric response function called also the *Bethe* surface of the target material.

5- The dielectric response function of liquid water

$$\eta_2(E,0) = Im\left[-1/\varepsilon(E,0)\right]$$

$$\varepsilon(E,K) = \varepsilon_1(E,K) + i\,\varepsilon_2(E,K)$$

Real Part for K = 0:

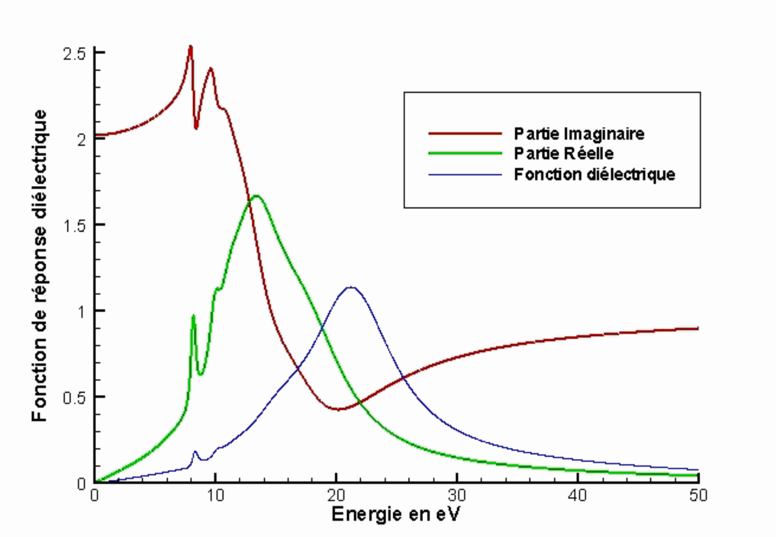
$$\varepsilon_{1,Exc}(E,0) = 1 + E_P^2 \sum_j^{exc} f_j \frac{(E_j^2 - E^2)[(E_j^2 - E^2)^2 + 3(\gamma_j E)^2]}{[(E_j^2 - E^2)^2 + (\gamma_j E)^2]^2}$$

$$\varepsilon_{1,Ioni}(E,0) = 1 + E_P^2 \sum_j^{Ioni} f_j \frac{E_j^2 - E^2}{(E_j^2 - E^2)^2 + (\gamma_j E)^2}$$

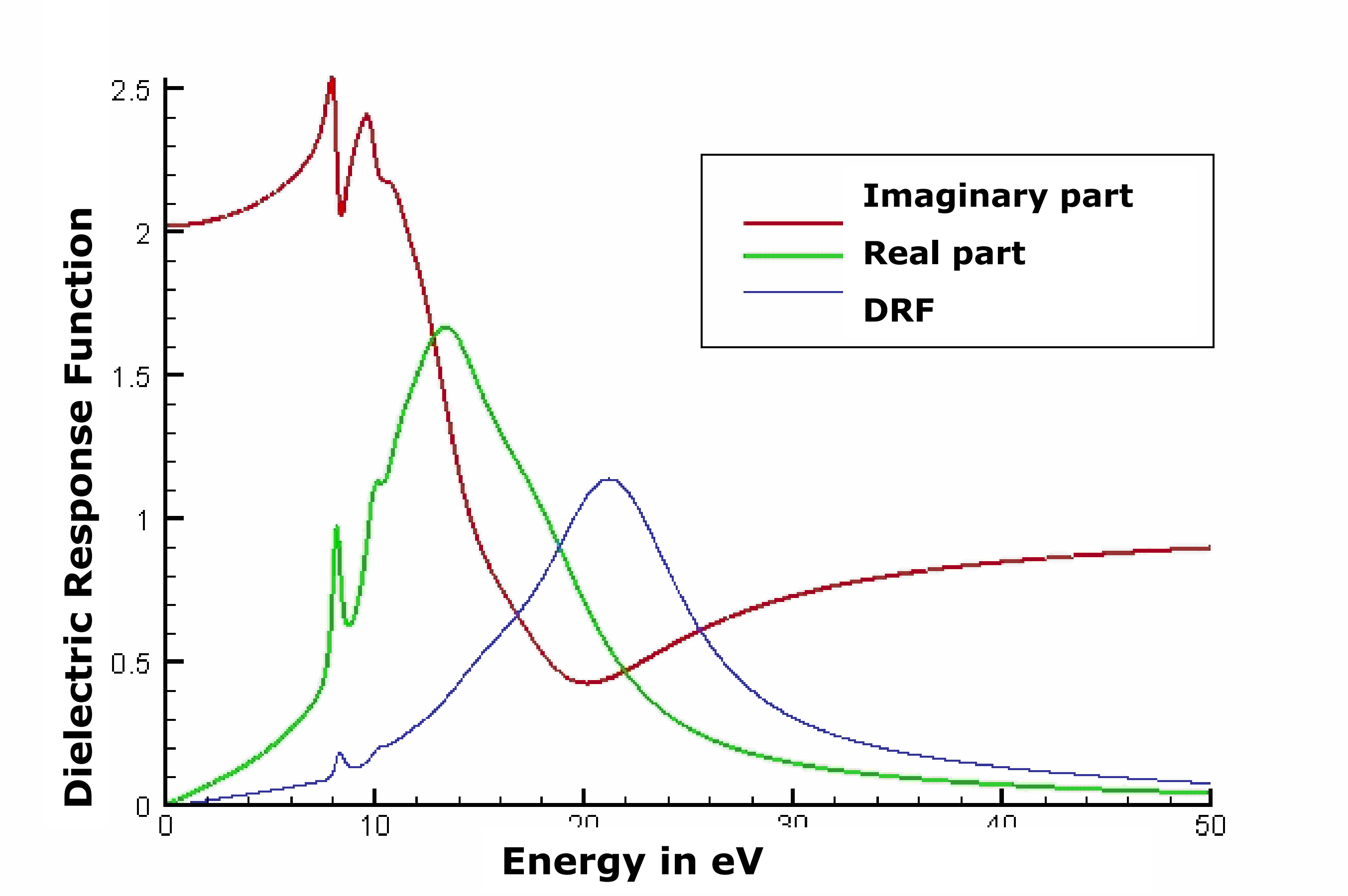
Imaginary part for K = 0:

$$\varepsilon_{2,Exc}(E,0) = E_P^2 \sum_j^{exc} f_j \frac{2(\gamma_j E)^3}{[(E_j^2 - E^2)^2 + (\gamma_j E)^2]^2}$$

$$\varepsilon_{2,Ioni}(E,0) = E_P^2 \sum_j^{Ioni} f_j \frac{\gamma_j E}{(E_j^2 - E^2)^2 + (\gamma_j E)^2}$$



The dielectric response function of liquid water for k = 0



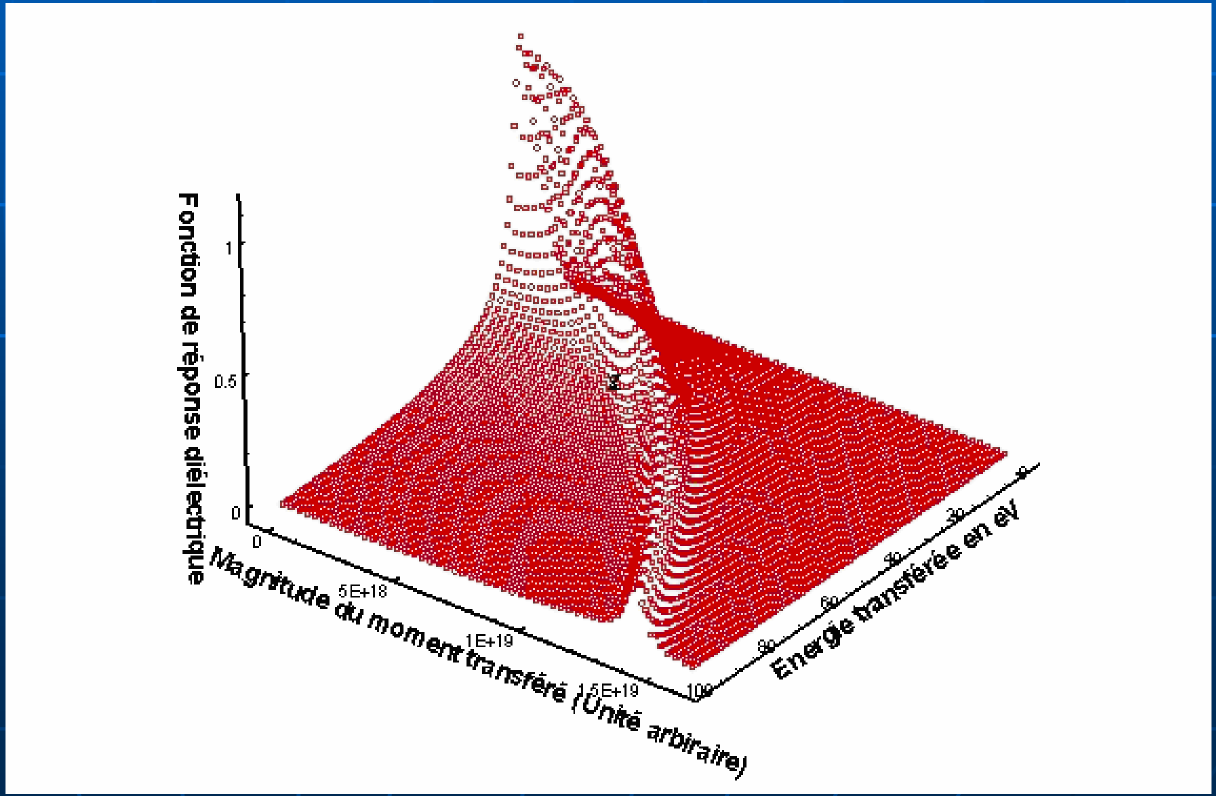
The dielectric response function of liquid water K > 0

Dispersion to momentum transfer k > 0 :

$$f_{j,exc}(K) = f_{j,exc}(e^{-a_j K^2} + b_j K^2 e^{-c_j K^2})$$

$$E_{j,Ioni}(q) = E_{j,Ioni} + \frac{q^2}{2m}$$

$$f_{j,Ioni}(K) = f_{j,Ioni} \frac{1 - \sum_j^{exc} f_{j,exc}(K)}{1 - \sum_j^{exc} f_{j,exc}}$$

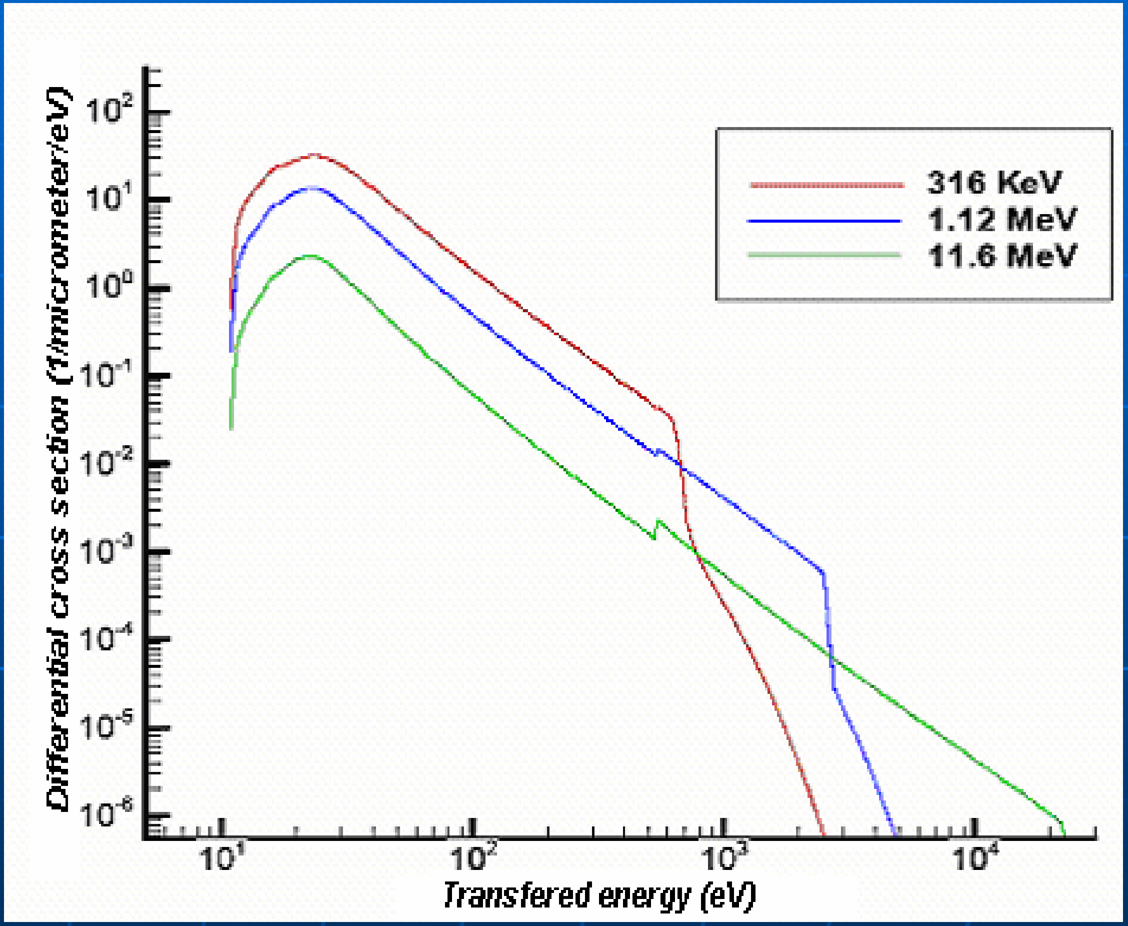


6- Calculation results

$$\frac{d\Sigma}{dE} = \int_{K\,min}^{K\,max} \frac{d^2\Sigma}{dE.dK}\,\frac{dK}{K}$$

$$K_{min} = \frac{\sqrt{2M}}{\hbar}\left(\sqrt{\tau} - \sqrt{\tau - E}\right)$$

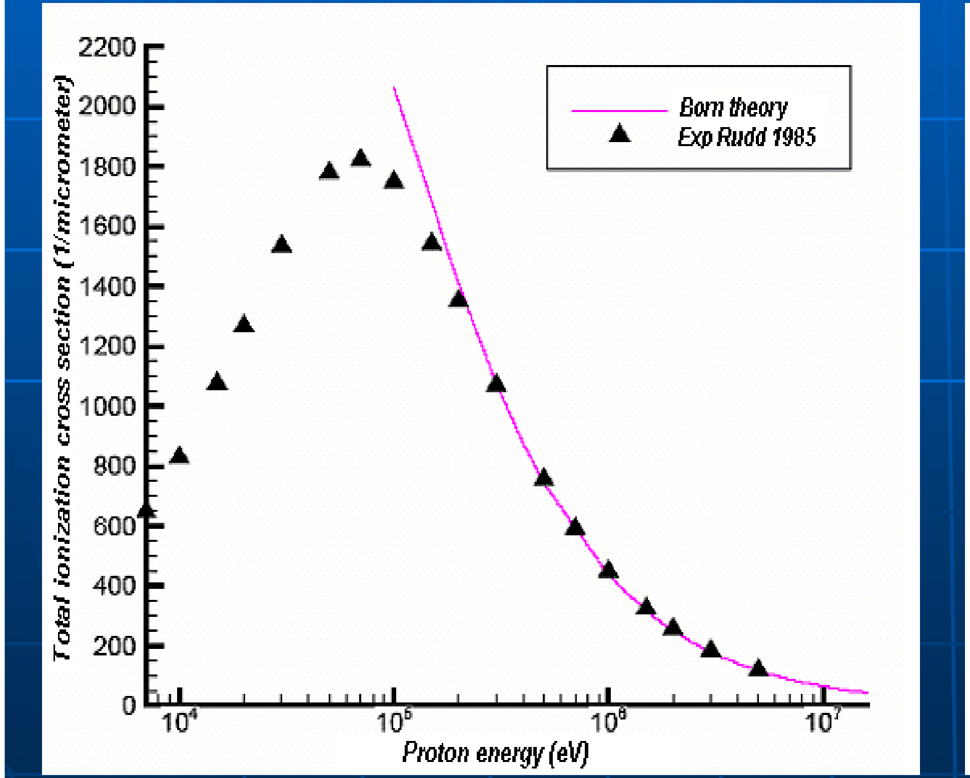
$$K_{max} = \frac{\sqrt{2M}}{\hbar}\left(\sqrt{\tau} + \sqrt{\tau - E}\right)$$

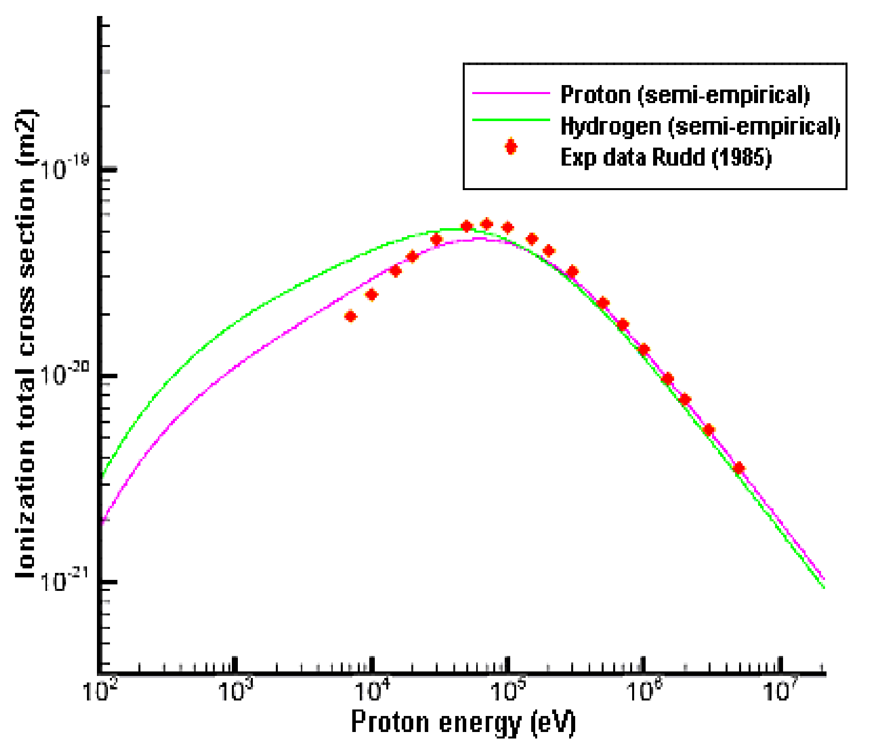


Protons ionization single differential cross section

Protons total ionization cross section

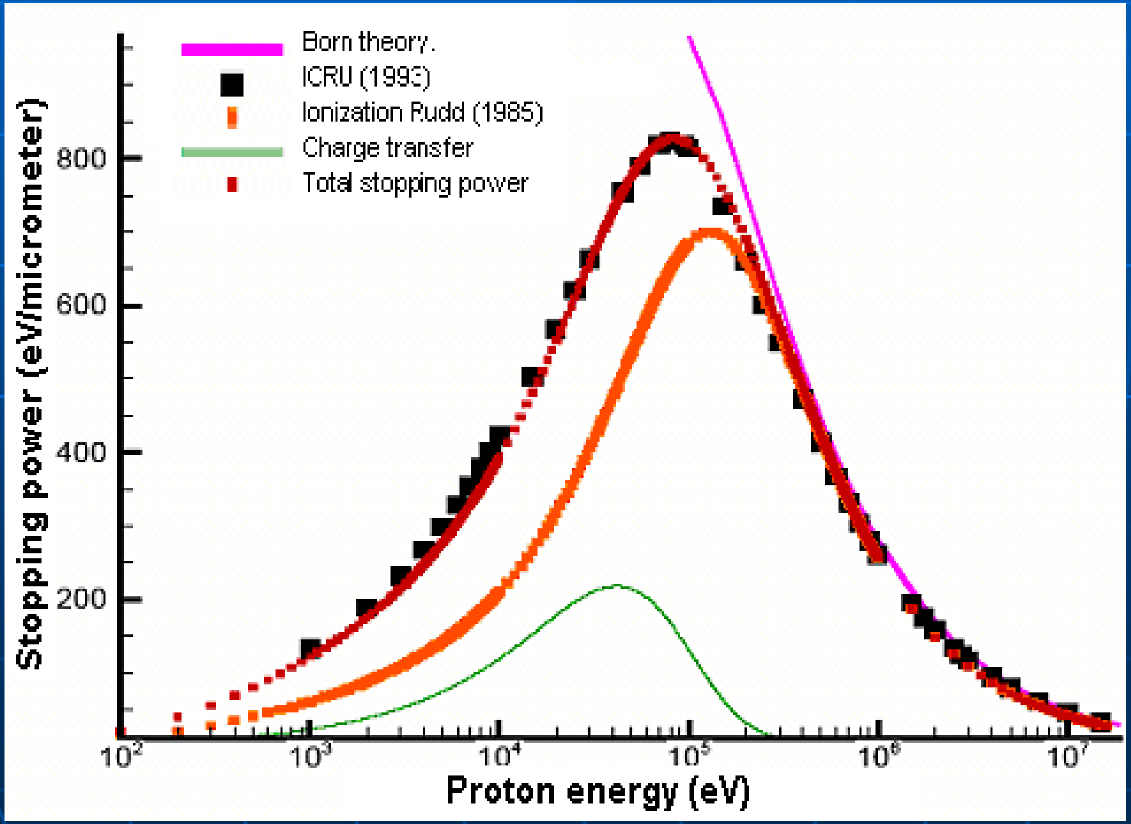
$$\Sigma = \int_{0}^{E\,max} \frac{d\Sigma}{dE} dE = \int_{0}^{E\,max} \int_{k\,min}^{k\,max} \frac{d^2\Sigma}{dE.dK} \frac{dK}{K} dE$$



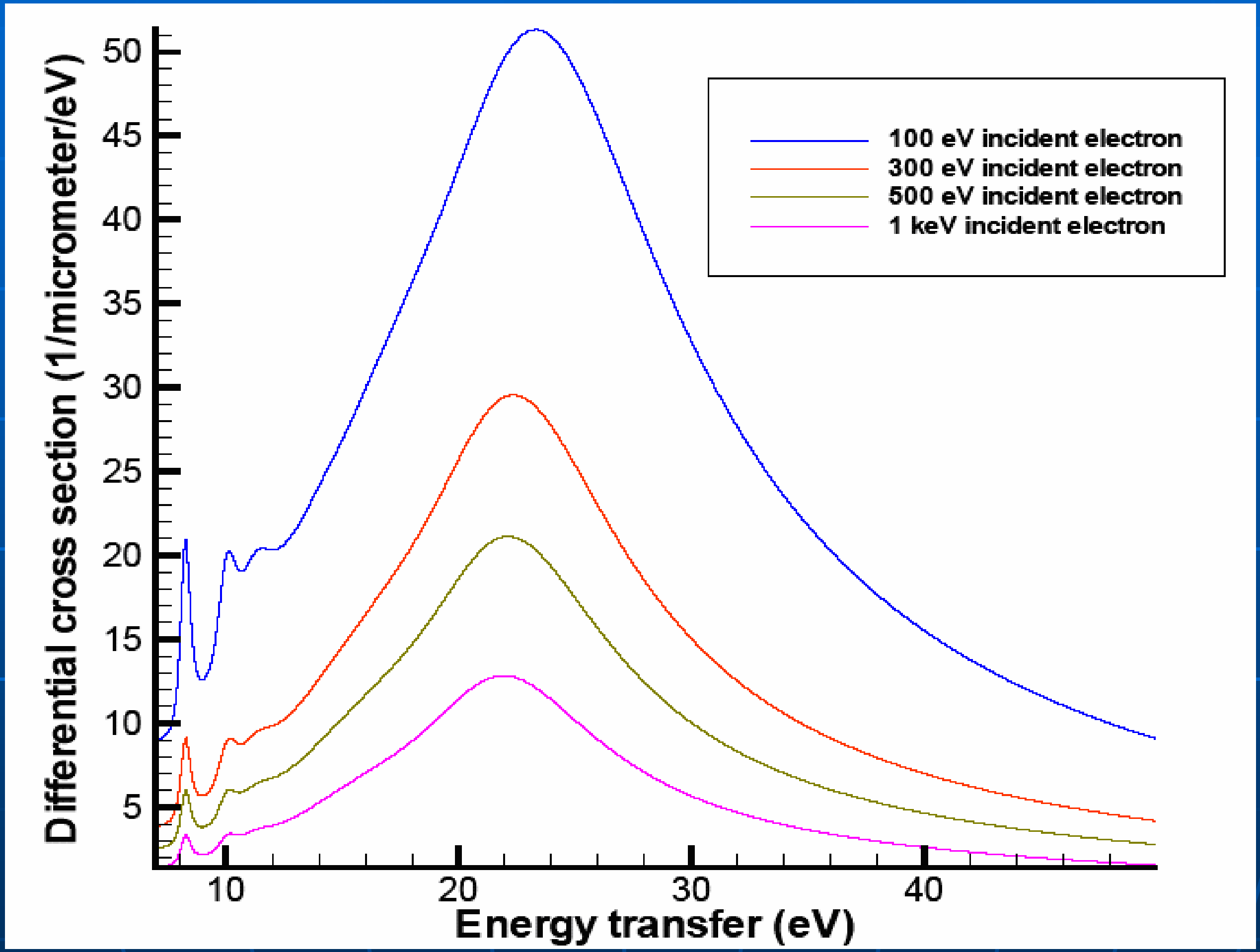


Stopping power for protons in water

$$\frac{dE}{dX} = \int_{0}^{E\,max} E \frac{d\Sigma}{dE} dE$$



Electrons Inelastic differential cross section



Inelastic differential cross section for incident electrons in water, for *1keV*, *500eV*, *300eV*, and *100eV* kinetic energies.

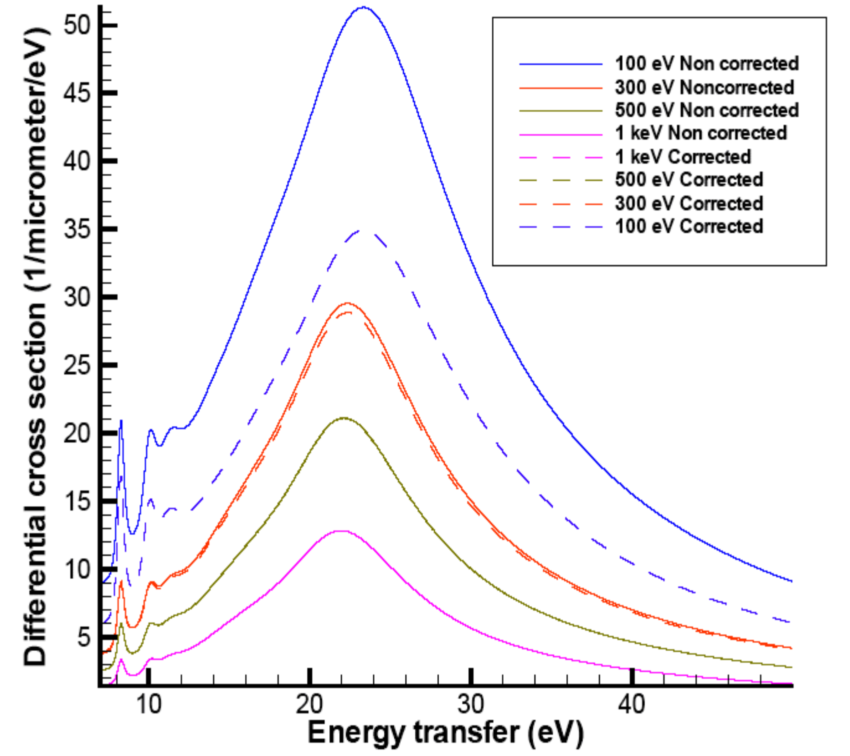
Electron's cross section corrections at low energies

Paretzke's correction :

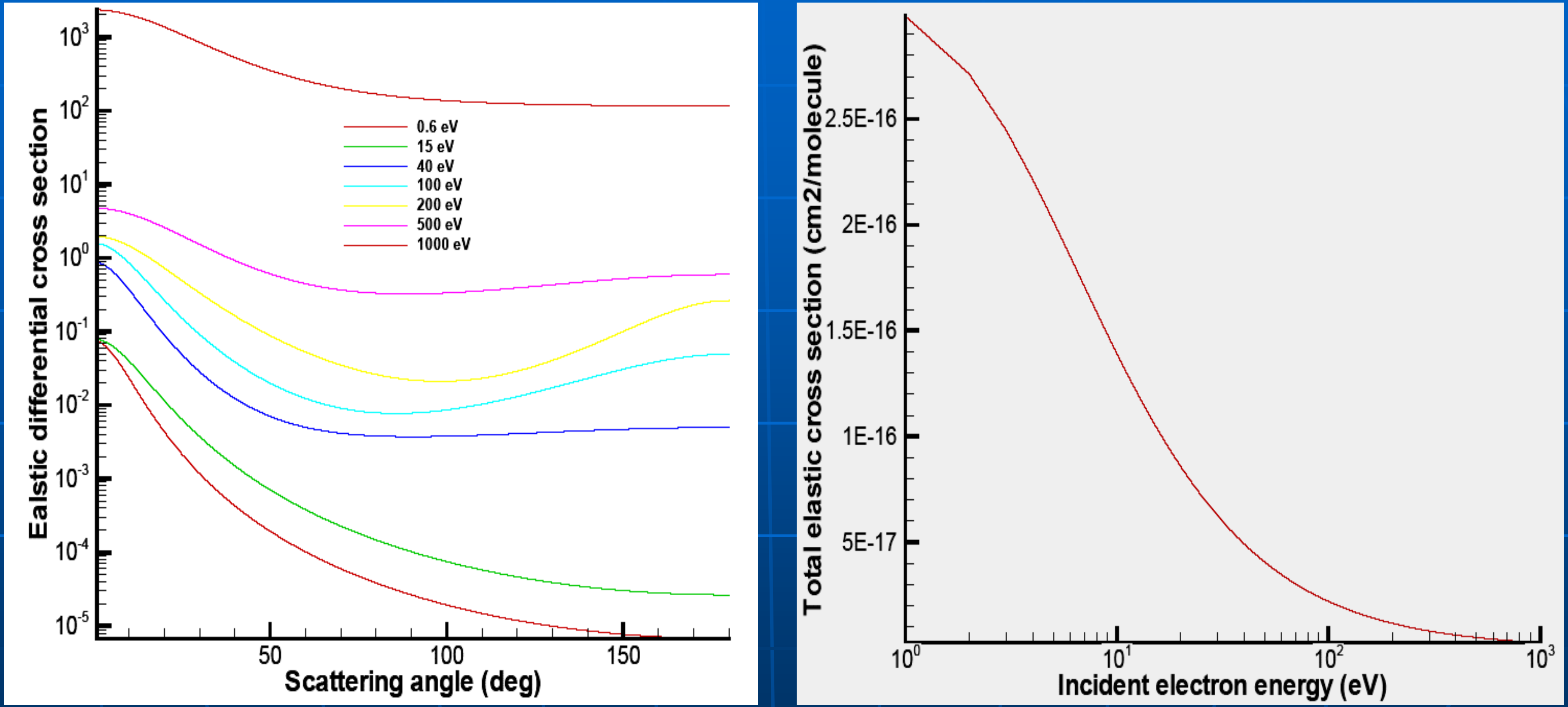
$$\frac{d\Sigma}{dE} = \sum_j \Phi_j(T)\frac{d\Sigma_j}{dE}$$

$$\Phi_j = 1 - exp[d_j(T/E_j - 1)] \quad \text{for} \quad T > E_j$$

$$\Phi_j = 0 \quad \text{for} \quad T \le E_j$$

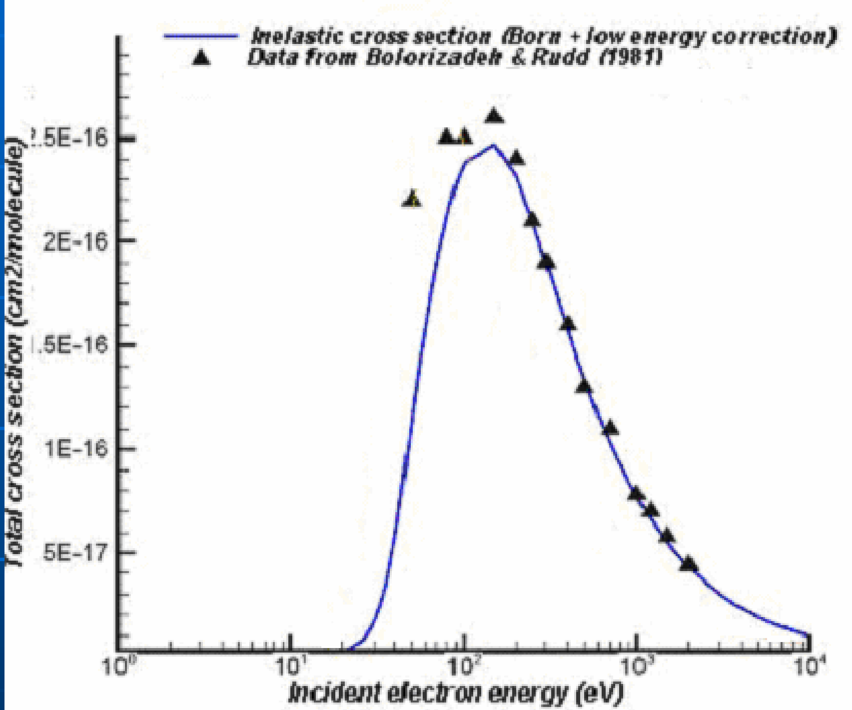


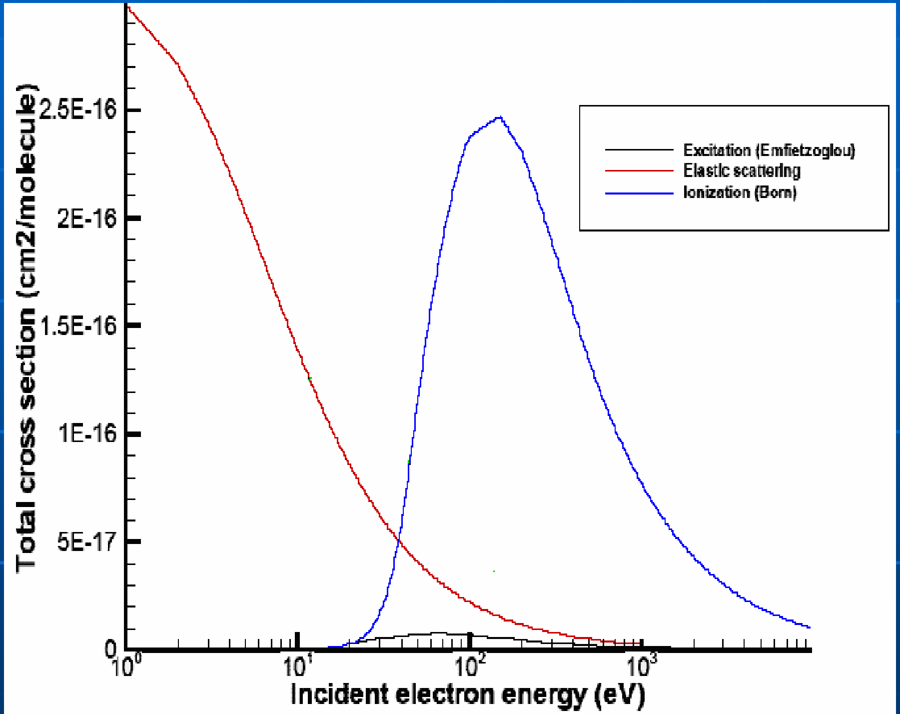
Electrons elastic scattering cross section



Electrons elastic scattering cross section for different incident kinetic energies.

Total cross section for incident electrons in water





Total ionization cross section for electrons in water compared to experimental data of *Bolorizadeh & Rudd (1981)* and to the elastic scattering cross section and also to the excitation cross section

7- Concluding remarks

- Electrons correction terms should be reviewed
- Calculated cross sections should be validated and compared to experimental data.
- Implemented processes should be tested on different machines.
- With these processes we should be able to estimate the energy deposed in the cell or even in the DNA molecule (nanometer scale).
- These processes are very time consuming which makes them useless at the macroscopic scale.