Electron interaction physics models in DNA Bases

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Motivation

- Generally, the biological medium in Monte Carlo track structure code is liquid water.
- In CPA100 code (developed in Toulouse till 2008, but no more maintained),
  - physics models for electron in liquid water and the 4 DNA bases are defined,
  - to simulate direct and indirect DNA damages (physical and chemical stages)
- The CPA100 physics models for liquid water has already been implemented in Geant4-DNA (option6) for
  - the three processes (elastic, excitation, ionisation)
  - over the 11 eV – 256 keV
  - as an alternative option.
  - some CPA100 cross sections data are in a better agreement with published data

Implementation of electron physics models in DNA bases following the same procedure as in CPA100 code but with more recent data and over a large energy range (-> 1 MeV)

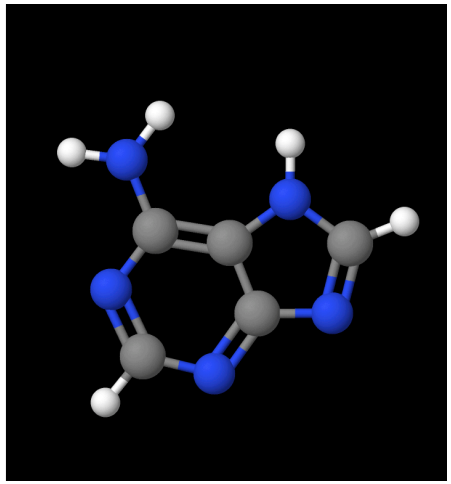
Goals

- Elastic scattering (IAM) with ELSEPA (Dirac partial wave analysis)
  - Angular differential
  - Integrated
- Ionization (BEB model, including relativistic correction)
  - Energy differential for each molecular orbital,
  - Integrated for each molecular orbital
  - Total
- Excitation

DNA Bases

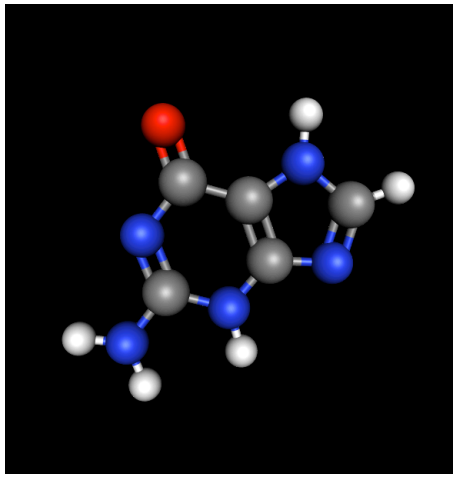
- Structure

Adenine: C5N5H5



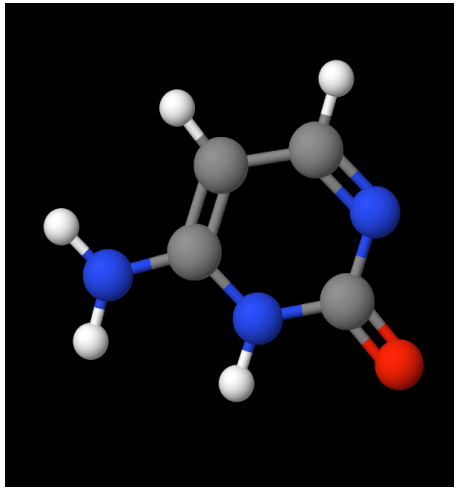
70 electrons
10 inner shells
25 valence shells
A= 135,13 g

Guanine: C5N5OH5



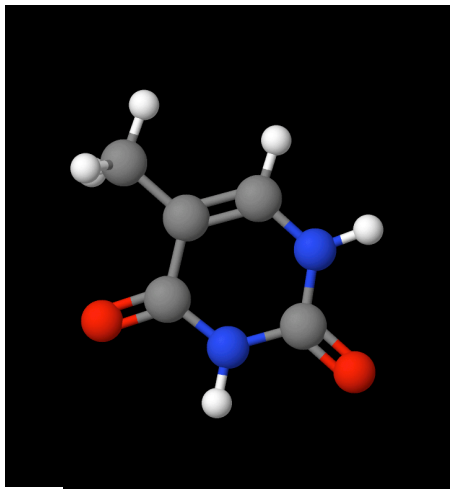
78 electrons
11 inner shells
28 valence shells
A= 151,13 g

Cytosine: C4N3OH5



58 electrons
8 inner shells
21 valence shells
A= 111,10 g

Thymine: C5N2O2H6



66 electrons
9 inner shells
24 valence shells
A= 126,11 g

Elastic scattering

(Mott & Massey, 1965, The theory of atomic collisions

- Independant Atom Model (Mott and Massey)
  - Differential cross section

$$\frac{d\sigma}{d\Omega} = \sum_{i=1}^{N} \left(\frac{d\sigma^A}{d\Omega}\right)_i + \sum_{i \neq j \neq 1}^{N} \frac{\sin(sr_{ij})}{sr_{ij}} \left[f_i(\theta) f_j^*(\theta) + g_i(\theta) g_j^*(\theta)\right]$$

Distance

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2$$

Scattering amplitude

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \{(l+1)\left[\exp(2i\delta_{l+}) - 1\right] + l\left[\exp(2i\delta_{l-}) - 1\right]\} P_l(\cos\theta)$$

$$g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \{\exp(2i\delta_{l-}) - \exp(2i\delta_{l+})\} P_l^1(\cos\theta)$$

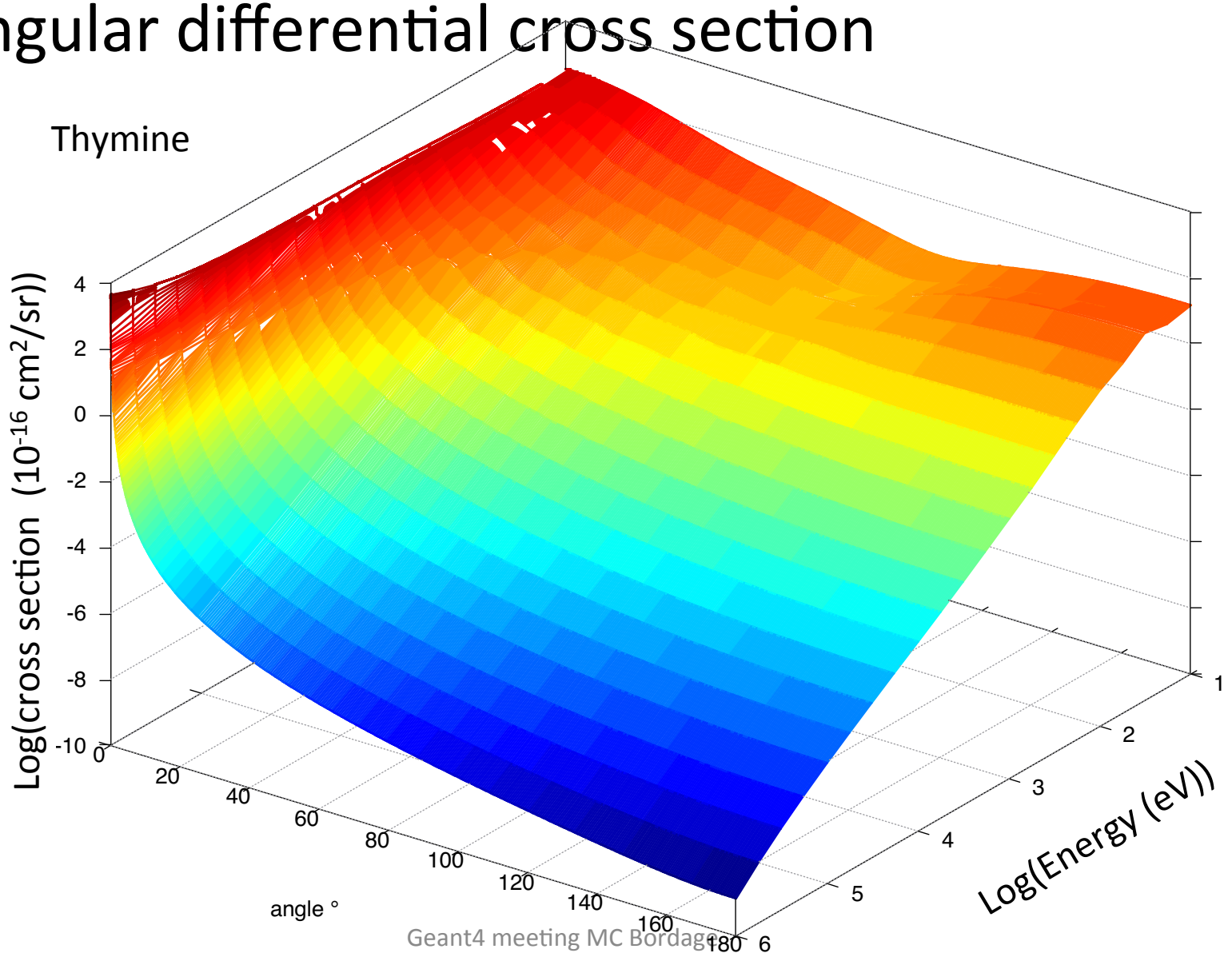
  - Total cross section

  - We use ELSEPA package to perform partial wave calculations for atoms

(Salvat et al. 2005, Comp. Phys. Com. 165,153)

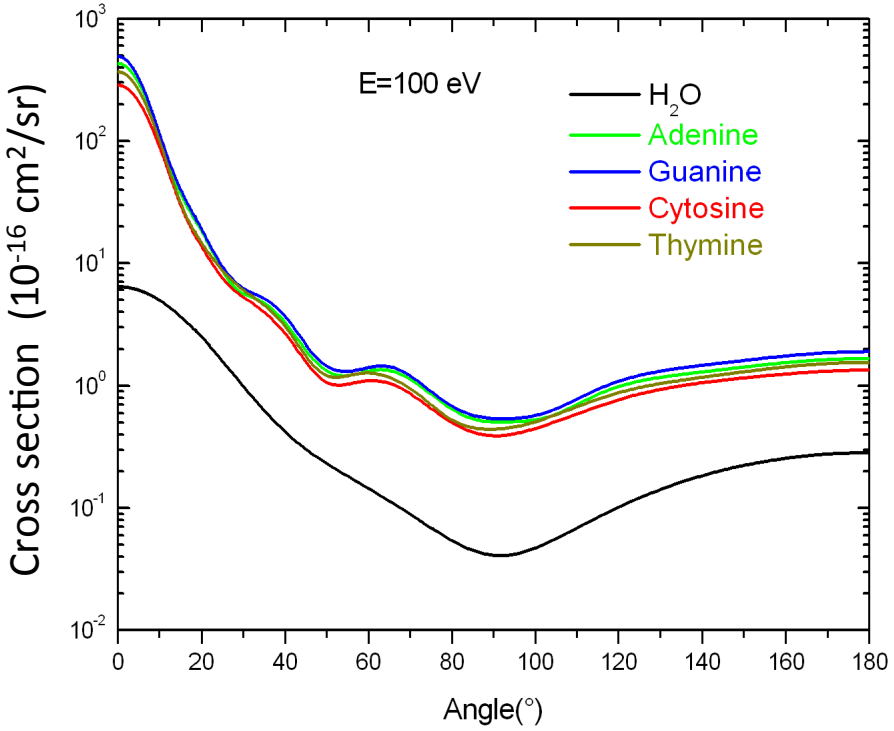
Elastic scattering

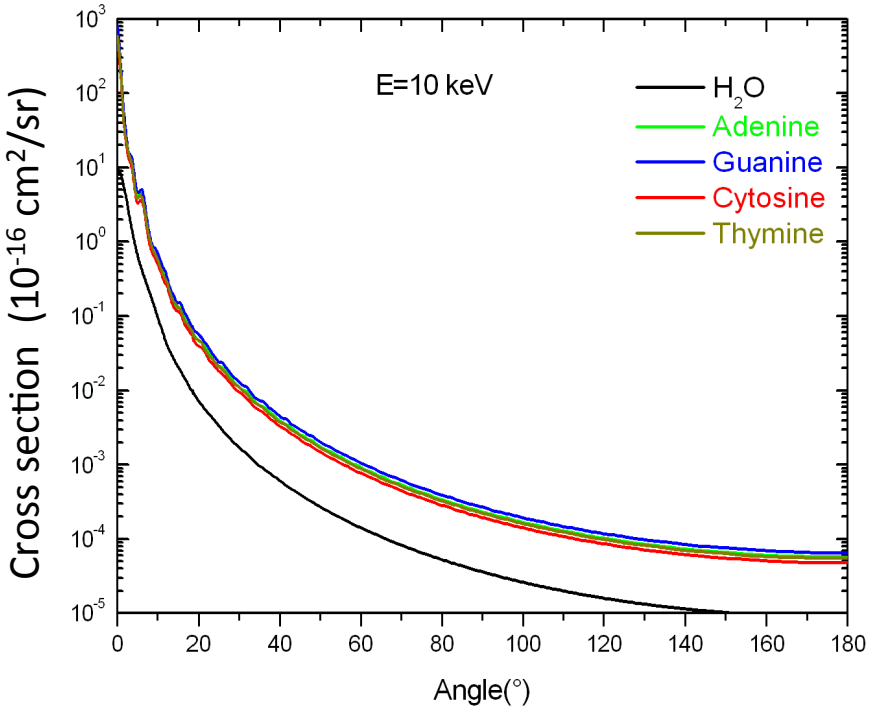
- Angular differential cross section



Elastic scattering

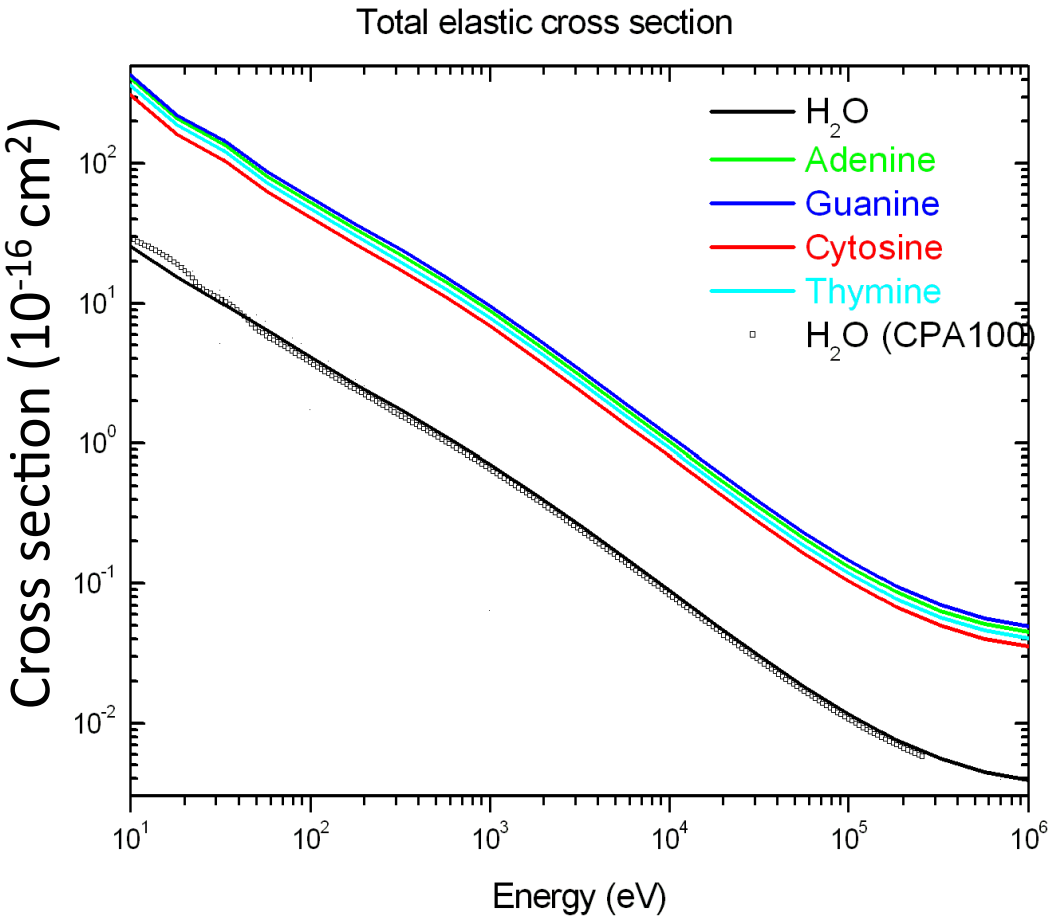
- Angular differential cross section



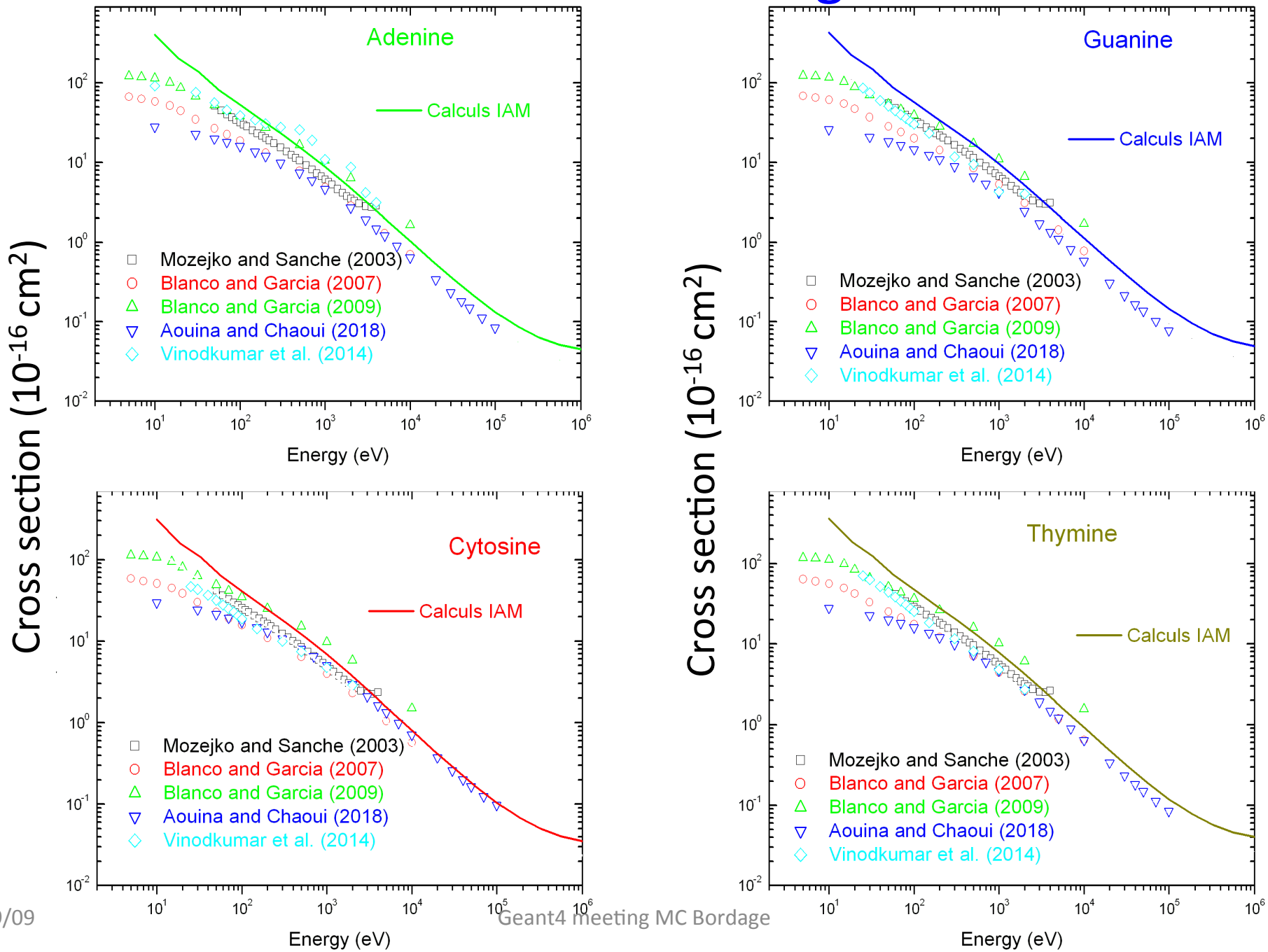


Elastic scattering

- Integrated cross section

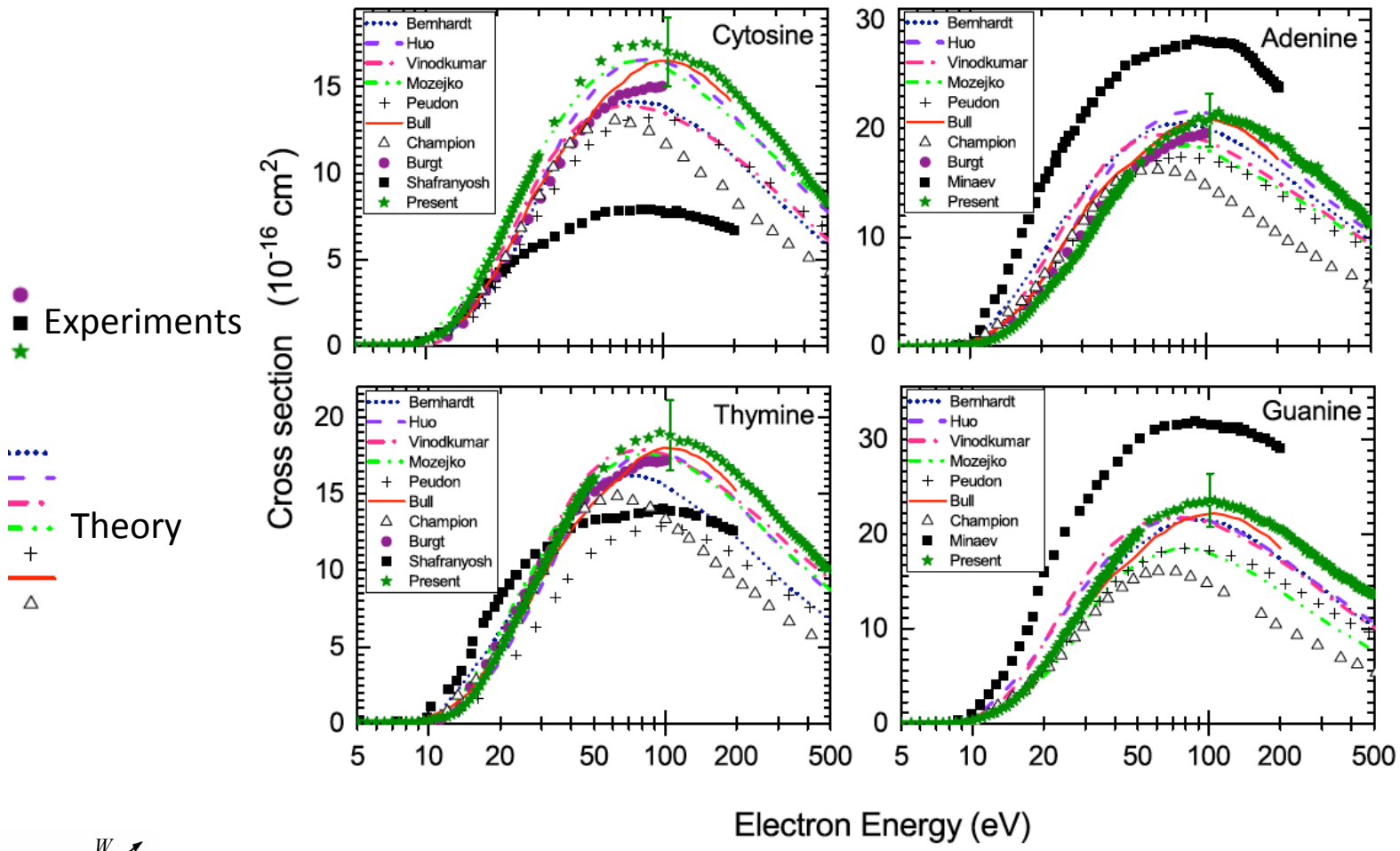


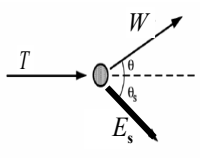
Elastic scattering



Ionization

- Ionization





Rahman et al., J. Chem. Phys. 2016

Ionization

(Guerra et al. 2015, J. Phys. B. 48,185202)

- Differential cross section for one shell (Relativistic Binary Encounter Bethe Vriens)

Orbital occupation number

$$\frac{d\sigma}{dw} = \frac{4\pi a_0^2 \alpha^4 N}{(\beta_t^2 + \beta_u^2 + \beta_b^2) 2b'} \left[\left(\frac{1}{(w+1)^2} + \frac{1}{(t-w)^2} + \frac{b'^2}{(1+0.5t')^2} \right) - \Phi_R \frac{1}{t+1} \left(\frac{1}{(w+1)} + \frac{1}{(t-w)} \right) \frac{1+2t'}{(1+0.5t')^2} + \left(Ln\left(\frac{\beta_t^2}{1-\beta_t^2}\right) - \beta_t^2 - Ln(2b') \right) \left(\frac{1}{(w+1)^3} + \frac{1}{(t-w)^3} \right) \right]$$

$$t = \frac{T}{B} \quad w = \frac{W}{B} \quad u = \frac{U}{B}$$

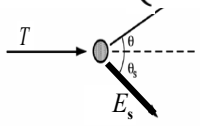
Electron kinetic energy

Binding energy

$$t' = \frac{T}{mc^2} \quad u' = \frac{U}{mc^2} \quad b' = \frac{B}{mc^2}$$

$$\Phi_R = cos\left[\sqrt{\frac{\alpha^2}{(\beta_t^2 + \beta_b^2)}} Ln\left(\frac{\beta_t^2}{\beta_b^2}\right) \right]$$

$$\beta_t^2 = 1 - \frac{1}{(1+t')^2} \quad et \; \beta_u^2 = 1 - \frac{1}{(1+u')^2} \quad \beta_b^2 = 1 - \frac{1}{(1+b')^2}$$



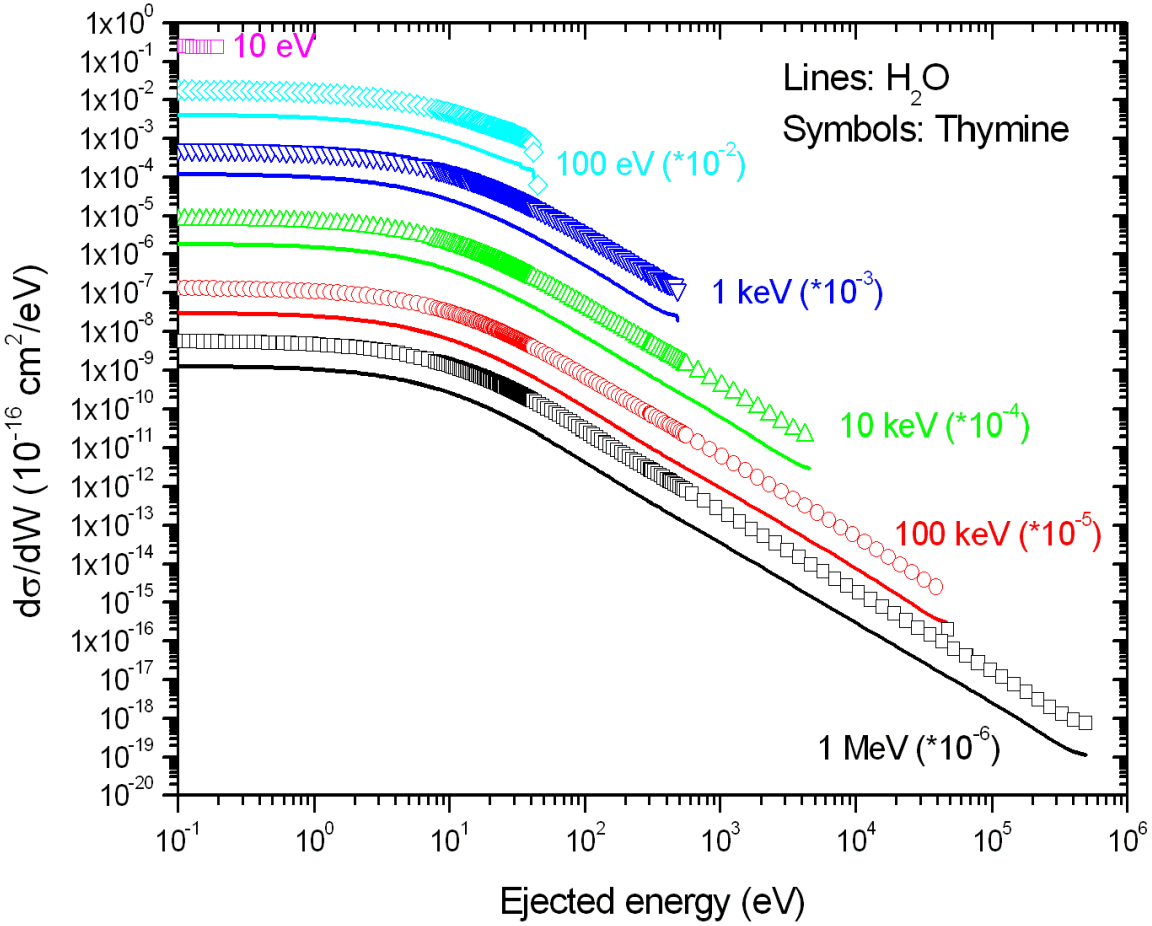
GAUSSIAN: A. Genoni, Univ Metz

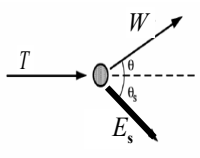
(Sakata et al. 2016, JAP 120,244901)

Ionization

- Ionization energy differential cross section: thymine

$$\left.\frac{d\sigma}{dw}\right]_{total} = \sum_{i=1}^{N\ MO} \left(\frac{d\sigma}{dw}\right)_i$$





Ionization

(Guerra et al. 2015, J. Phys. B. 48,185202)

- Total cross section for one shell (Relativistic Binary Encounter Bethe Vriens)

Bohr radius

$$\sigma = \frac{4\pi a_0^2 \alpha^4 N}{(\beta_t^2 + \beta_u^2 + \beta_b^2) 2b'} \left[\left(1 - \frac{1}{t} + \frac{t-1}{2} \frac{b'^2}{(1+0.5t')^2} \right) - \Phi_R \frac{Ln(t)}{t+1} \frac{1+2t'}{(1+0.5t')^2} + \frac{1}{2} \left(Ln\left(\frac{\beta_t^2}{1-\beta_t^2}\right) - \beta_t^2 - Ln(2b') \right) \left(1 - \frac{1}{t^2} \right) \right]$$

Fine-structure constant

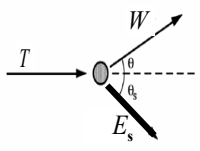
$$\Phi_R = cos \left[\sqrt{\frac{\alpha^2}{(\beta_t^2 + \beta_b^2)}} Ln\left(\frac{\beta_t^2}{\beta_b^2}\right) \right]$$

$$t = \frac{T}{B} \quad u = \frac{U}{B}$$

Electron kinetic energy

Binding energy

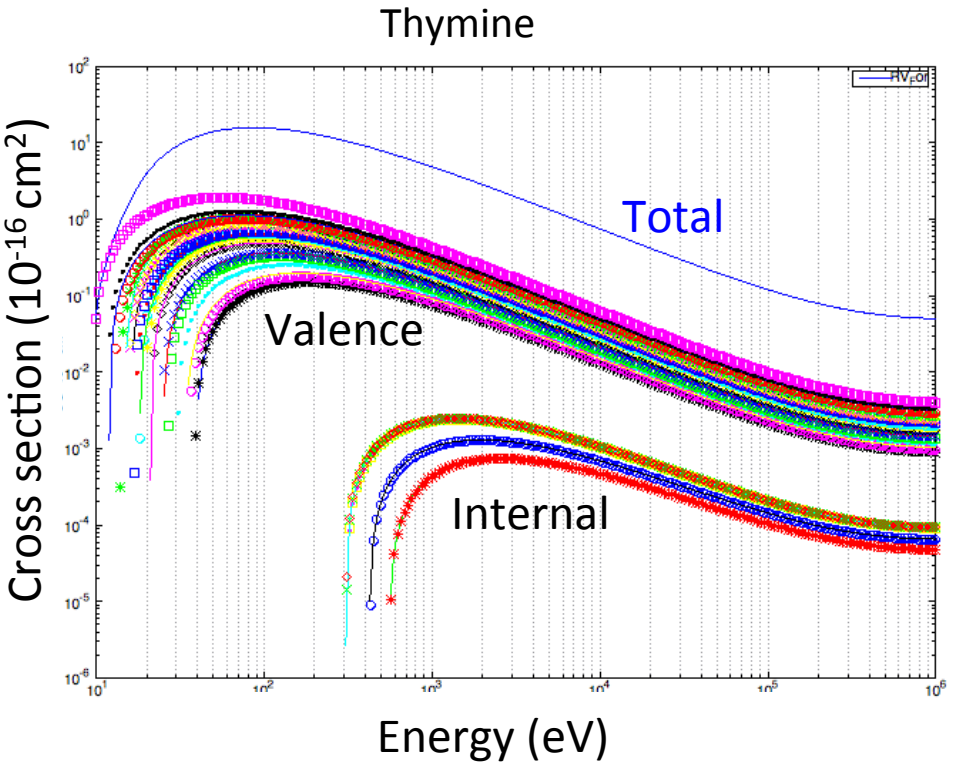
$$t' = \frac{T}{mc^2} \quad u' = \frac{U}{mc^2} \quad b' = \frac{B}{mc^2}$$

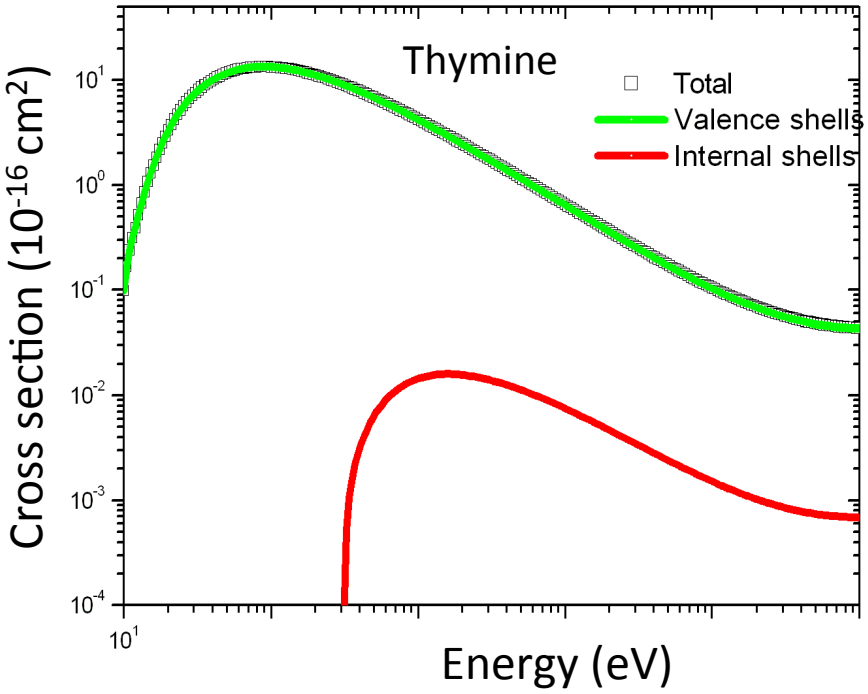


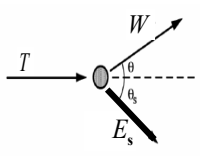
$$\beta_t^2 = 1 - \frac{1}{(1+t')^2} \quad et \ \beta_u^2 = 1 - \frac{1}{(1+u')^2} \quad \beta_b^2 = 1 - \frac{1}{(1+b')^2}$$

Ionization

- Total cross section for each shell



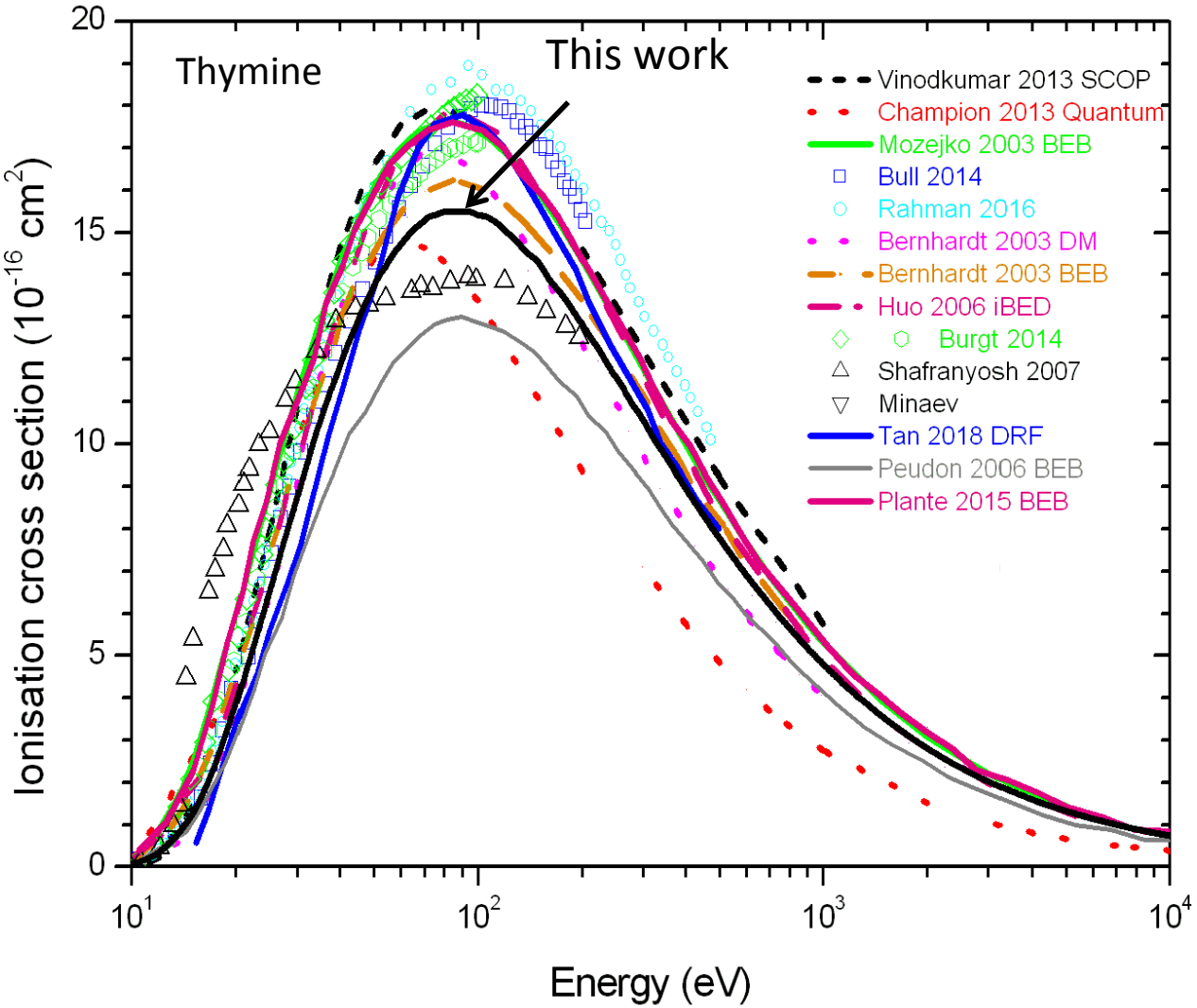


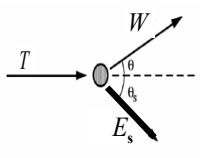


$$\sigma]_{total} = \sum_{i=1}^{N\ MO} (\sigma)_i$$

Ionization

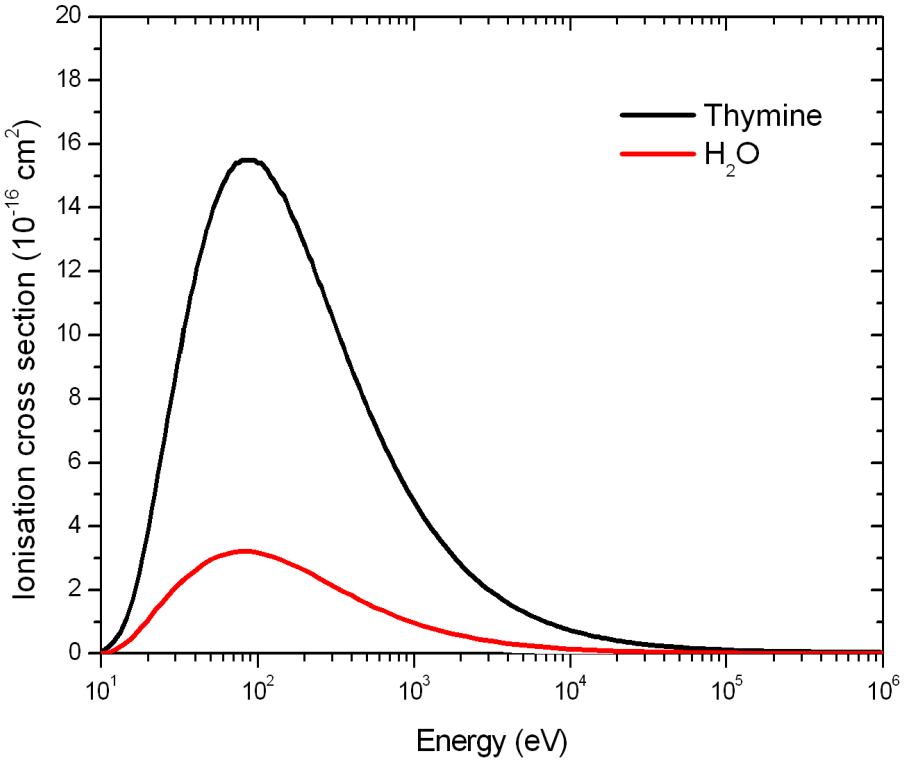
- Total

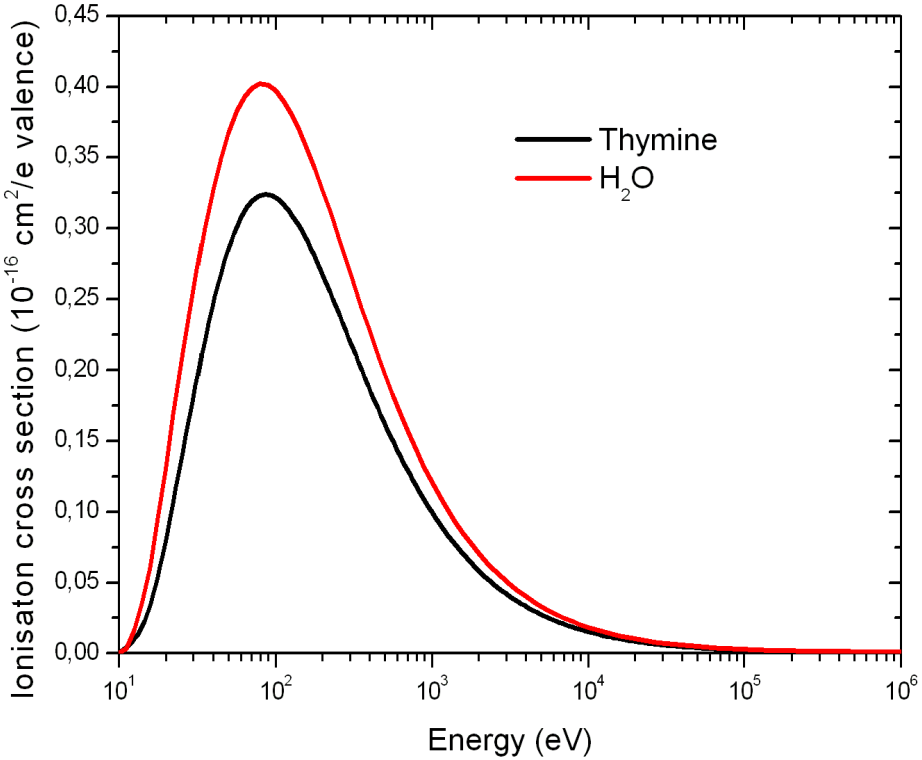


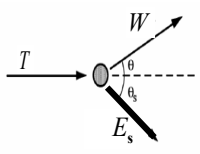


Ionization

- Total







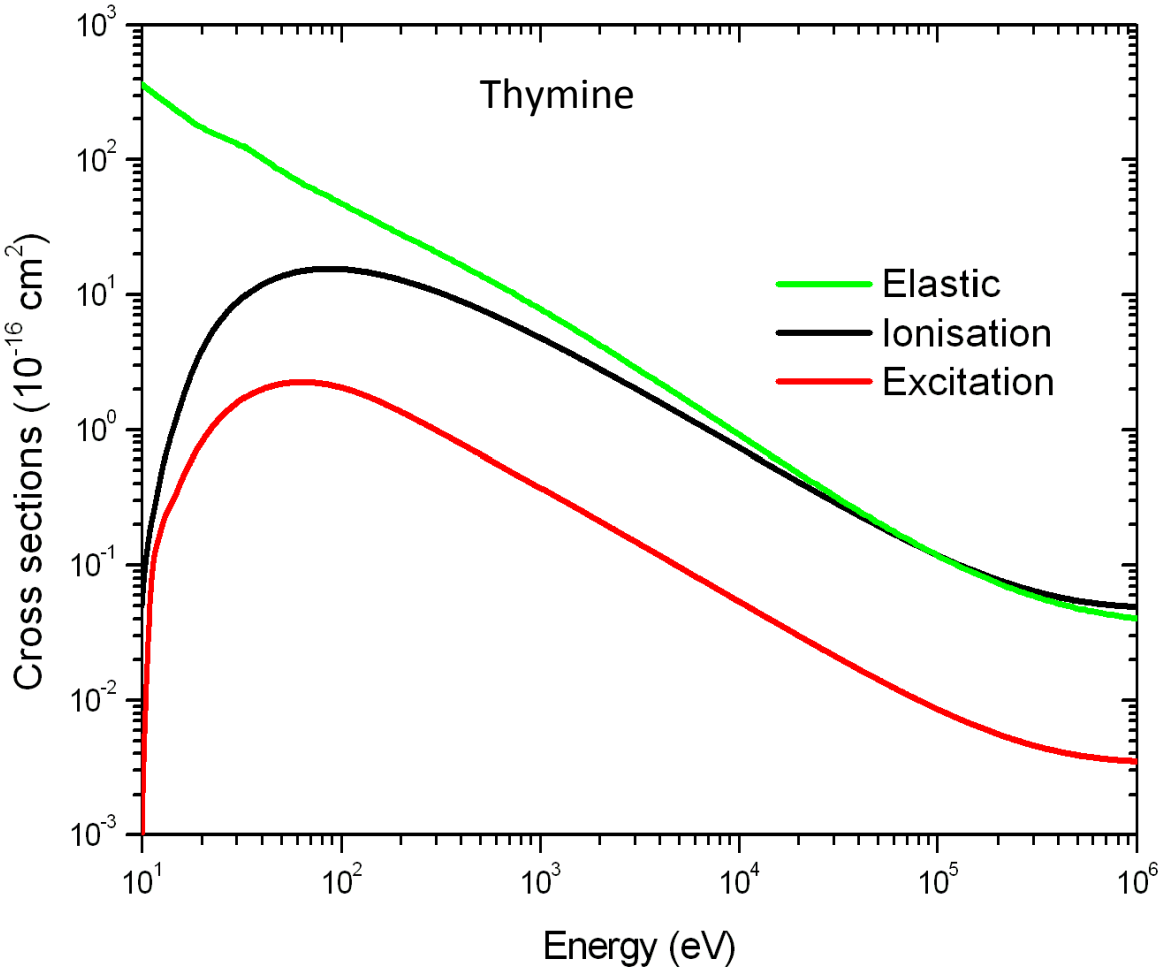
Excitation

- Hypothesis: $\left[\frac{\sigma_{exc}}{\sigma_{ion}}\right]_{DNA} = \left[\frac{\sigma_{exc}}{\sigma_{ion}}\right]_{H2O}$
- Dingfelder calculations: $\left[\frac{\sigma_{exc}}{\sigma_{ion}}\right]_{H2O}$ (Dingfelder et al. 1998, Rad. Phys. Chem.. 53,1-
  - Ratio is known in water
  - E>300 eV, this ratio -> constant (0.088)
- Total excitation cross section

$$[\sigma_{exc}]_{DNA} = [\sigma_{ion}]_{DNA} \left[\frac{\sigma_{exc}}{\sigma_{ion}}\right]_{H2O}$$

- Excitation if the ionization threshold < 20 eV

Cross section set for Thymine



Next stages

- Implementation of physics models (elastic, electronic excitation and ionisation) for 4 DNA bases in Geant4-DNA

- Verification of this implementation by the calculation of different parameters
  - number of interaction of each type
  - distances
  - stopping power ….

Thank you for your attention