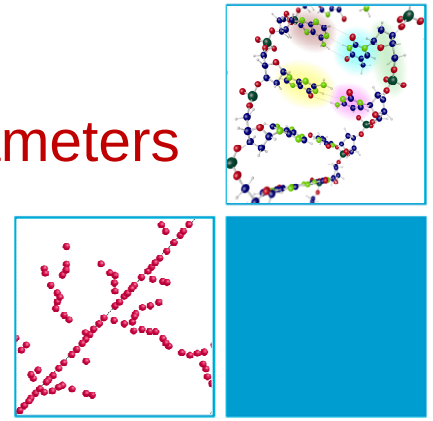
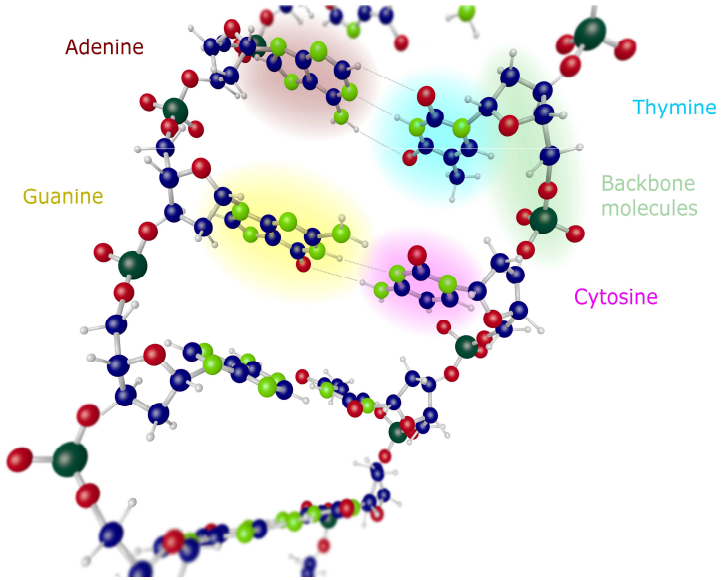
Simulation of electron tracks in water and DNA medium

Marion Bug

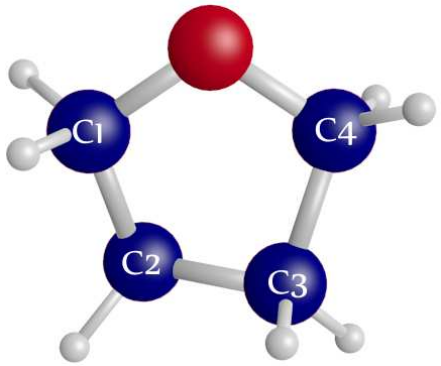
- How different are cross sections (CS) of water and DNA constituents for electrons with energies 7 eV – 1 keV?
- How sensitive are simulated track structure parameters to differences in CS data?



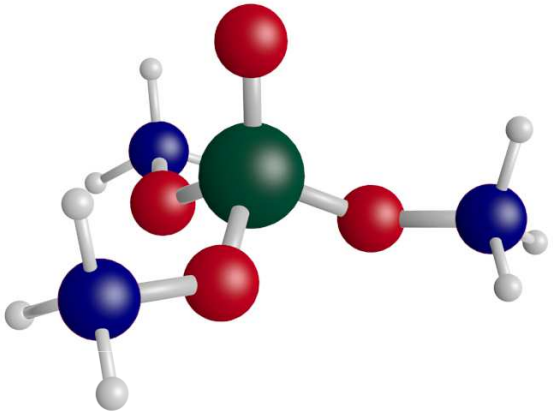
DNA constituents



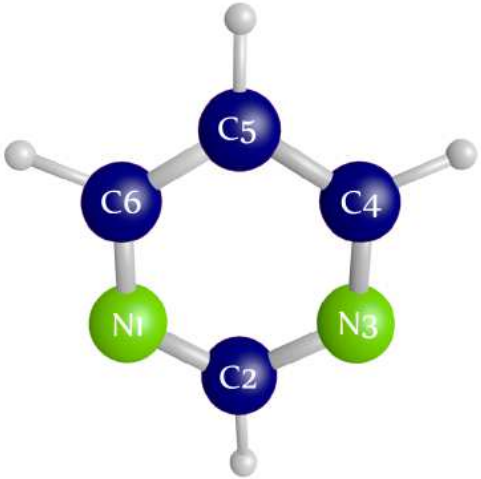
Tetrahydrofuran (THF)



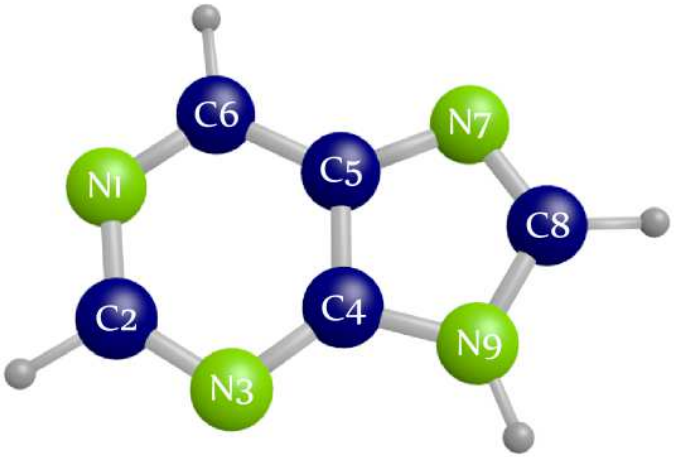
Trimethylphosphate (TMP)



Pyrimidine (PY)



Purine (PU)



Simulation of electron tracks

History of interactions is followed step by step

→ Path length

σ_t

→ Ionisation

σ_{ion} $\sigma_{ion,i}$

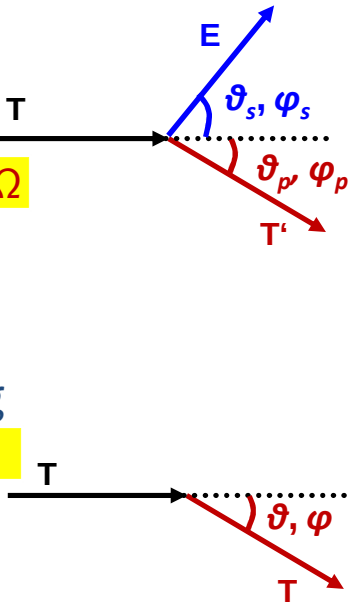
$d\sigma / dE$ $d^2\sigma / dE d\Omega$

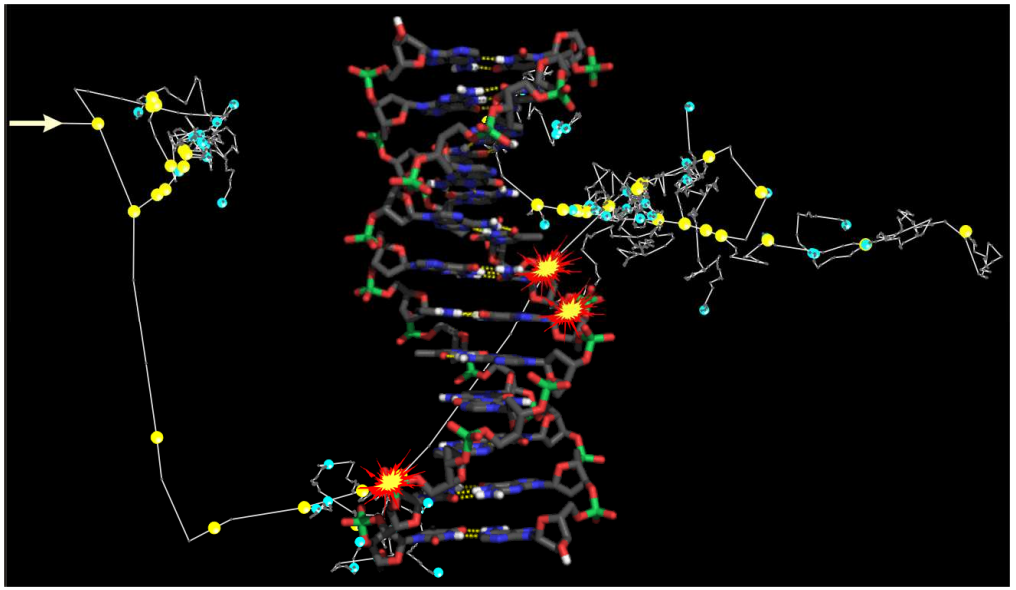
→ Excitation

σ_{exc} $\sigma_{exc,j}$

→ Elastic scattering

σ_{el} $d\sigma_{el} / d\Omega$





Accuracy of simulation results strongly depends on accuracy of interaction cross sections

Electron cross sections of DNA molecules

PTB
CENTRE FOR MEDICAL RADIATION PHYSICS

- Task:

  Development of model functions for a complete data set of CS for interaction of electrons ~7 eV – 1 keV with THF, TMP, PY und PU

- Requirements:
  - Physically reasonable interpolation of experimental data
  - Realististic extrapolation
  - Consistency

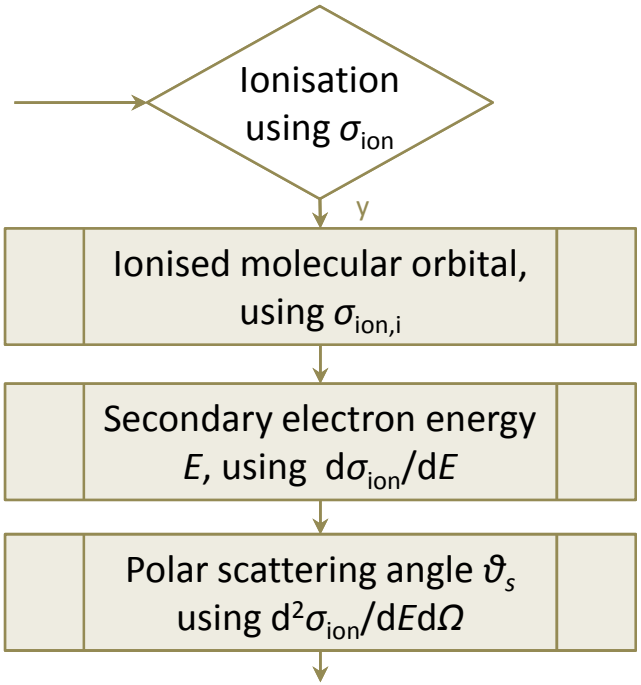
Data evaluation
Example: Ionisation-CS

PTB
CENTRE FOR MEDICAL RADIATION PHYSICS

Evaluation:

Experimental data as a function of
T, E und Ω

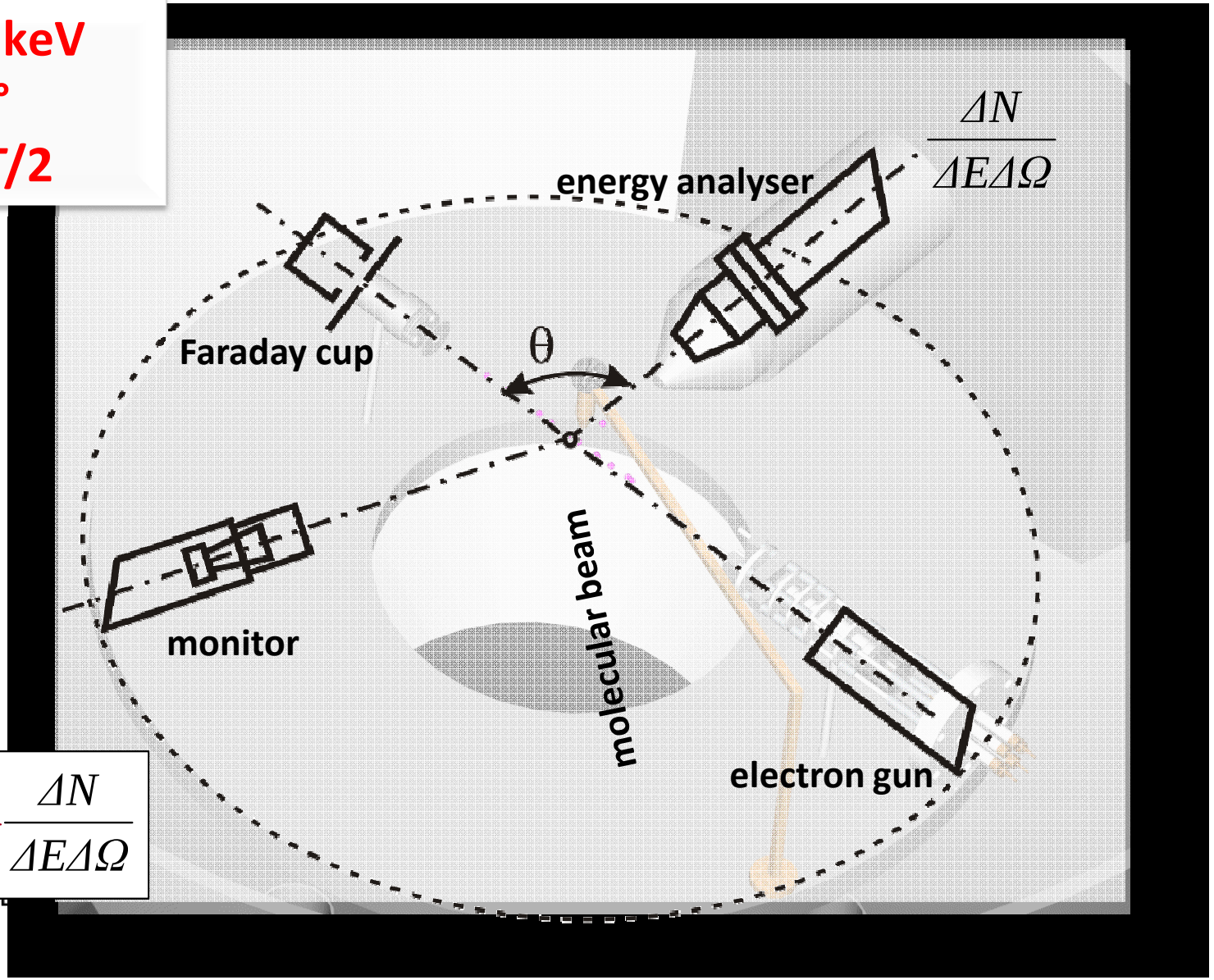
Simulation:



Measurement of differential CS

CENTRE FOR MEDICAL RADIATION PHYSICS

T: **20 eV – 1 keV**
Θ: **15° – 135°**
E: **2.7 eV – *T*/2**



$$\frac{d^2\sigma}{dEd\Omega} = \frac{\sigma_t}{\Delta I}\frac{e}{\eta(E)}\frac{\Delta N}{\Delta E \Delta \Omega}$$

Data evaluation
Example: Ionisation-CS

PTB
CENTRE FOR MEDICAL RADIATION PHYSICS

Evaluation:

Experimental data as a function of T, E und Ω

↓

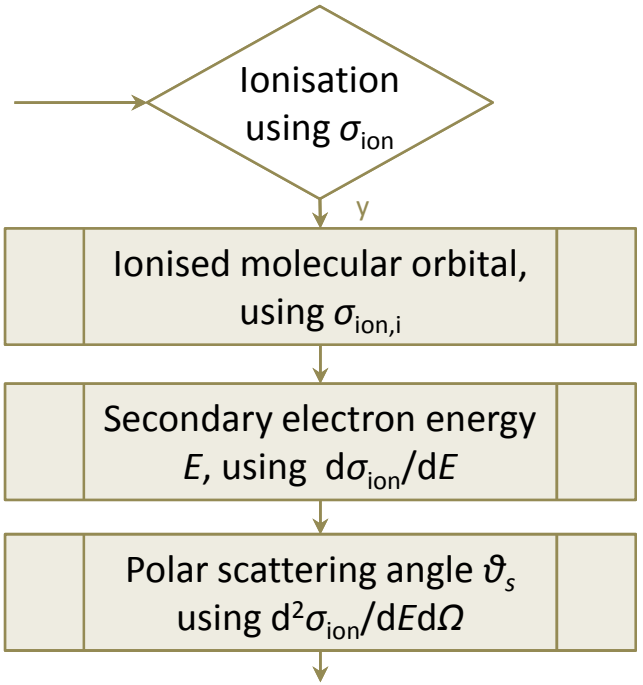
Fit of spline function as a function of E

↓

Fit of model function as a function of θ

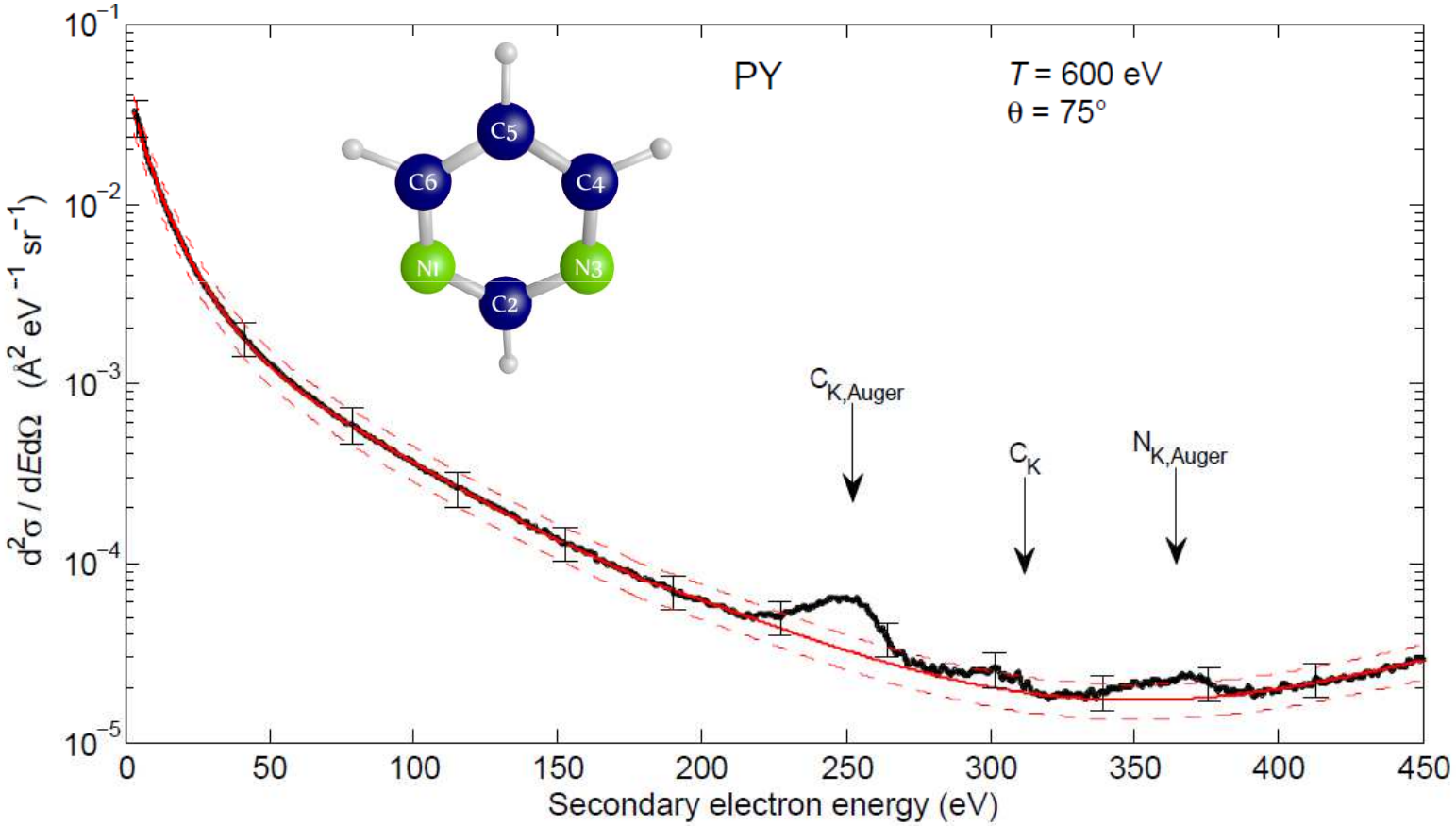
$d^2\sigma_{ion}/dEd\Omega$

Simulation:



Evaluation of measured DDCS

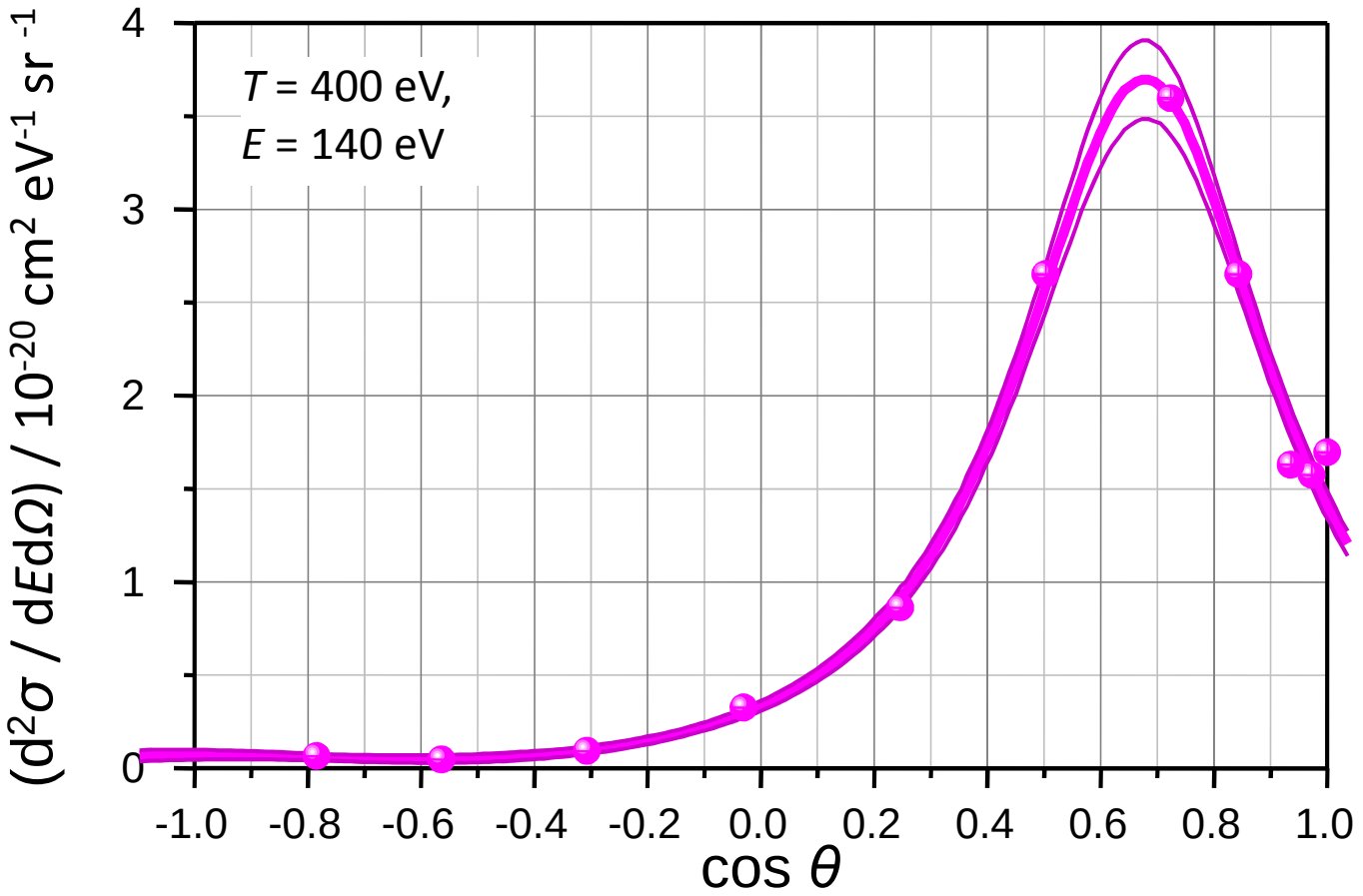
Fit of spline functions to
double-differential cross sections (DDCS)

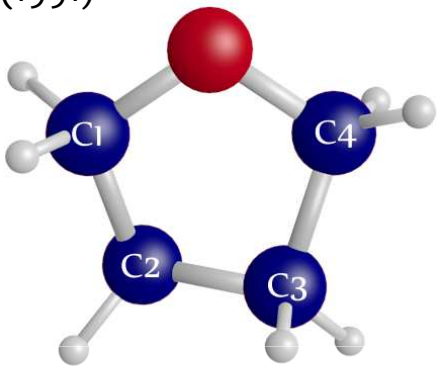


Model functions for DDCS

$$\frac{d^2\sigma}{dEd\Omega} = a\left[\frac{1}{1+\left(\frac{\cos\theta - b}{c}\right)^2} + \frac{d}{1+\left(\frac{\cos\theta + 1}{e}\right)^2}\right]^*$$

*Rudd et al., PRA 44 1644 (1991)

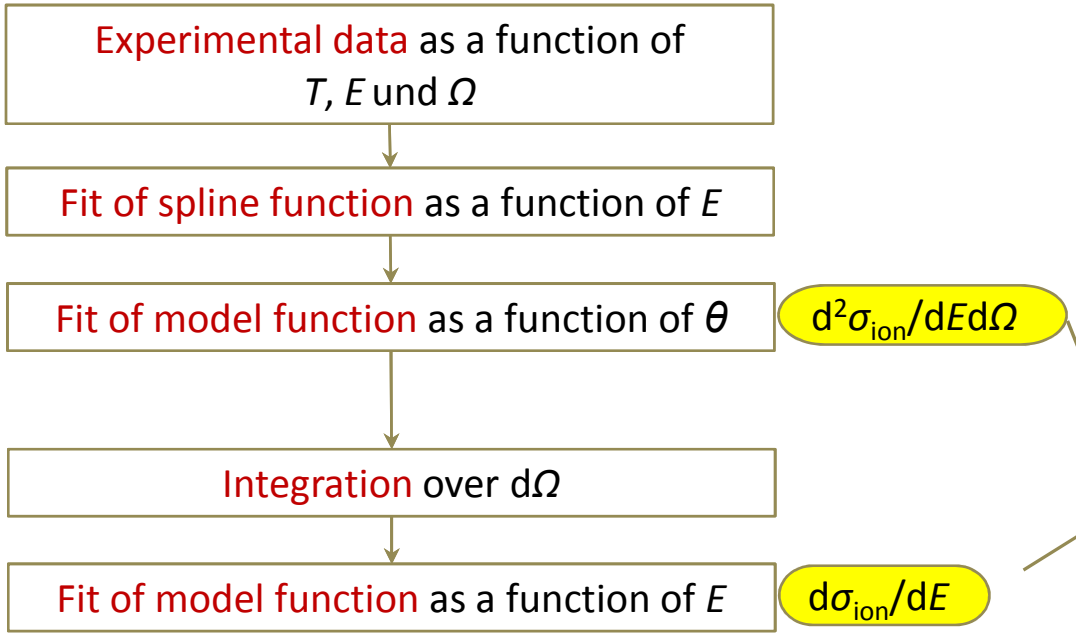




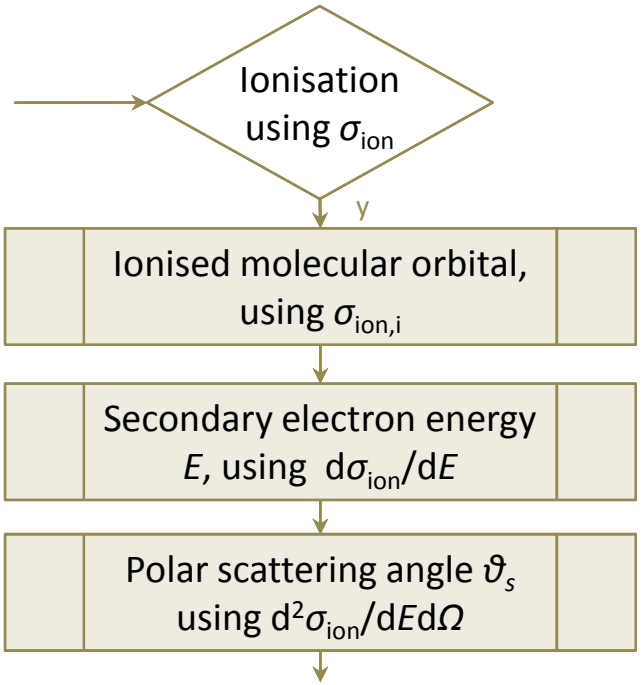
Data evaluation
Example: Ionisation-CS

PTB
CENTRE FOR MEDICAL RADIATION PHYSICS

Evaluation:



Simulation:



Single-differential ionisation CS

- By integration $$\frac{\mathrm{d}\sigma_{\mathrm{ion}}}{\mathrm{d}E}(T) = \int_0^{2\pi}\int_0^{\pi} \sin\theta \, \frac{\mathrm{d}^2\sigma}{\mathrm{d}E \, \mathrm{d}\Omega} \, \mathrm{d}\theta \, \mathrm{d}\varphi$$

- Fit of Binary-Encounter-Bethe model

$$\frac{\mathrm{d}\sigma_{\mathrm{ion}}}{\mathrm{d}E}(T) = \frac{P_1}{P_2\left(t'+P_3+1\right)} \sum_{n=1}^{3} F_n \left[f_n\left(w'\right) + f_n\left(t'-w'\right) \right]$$

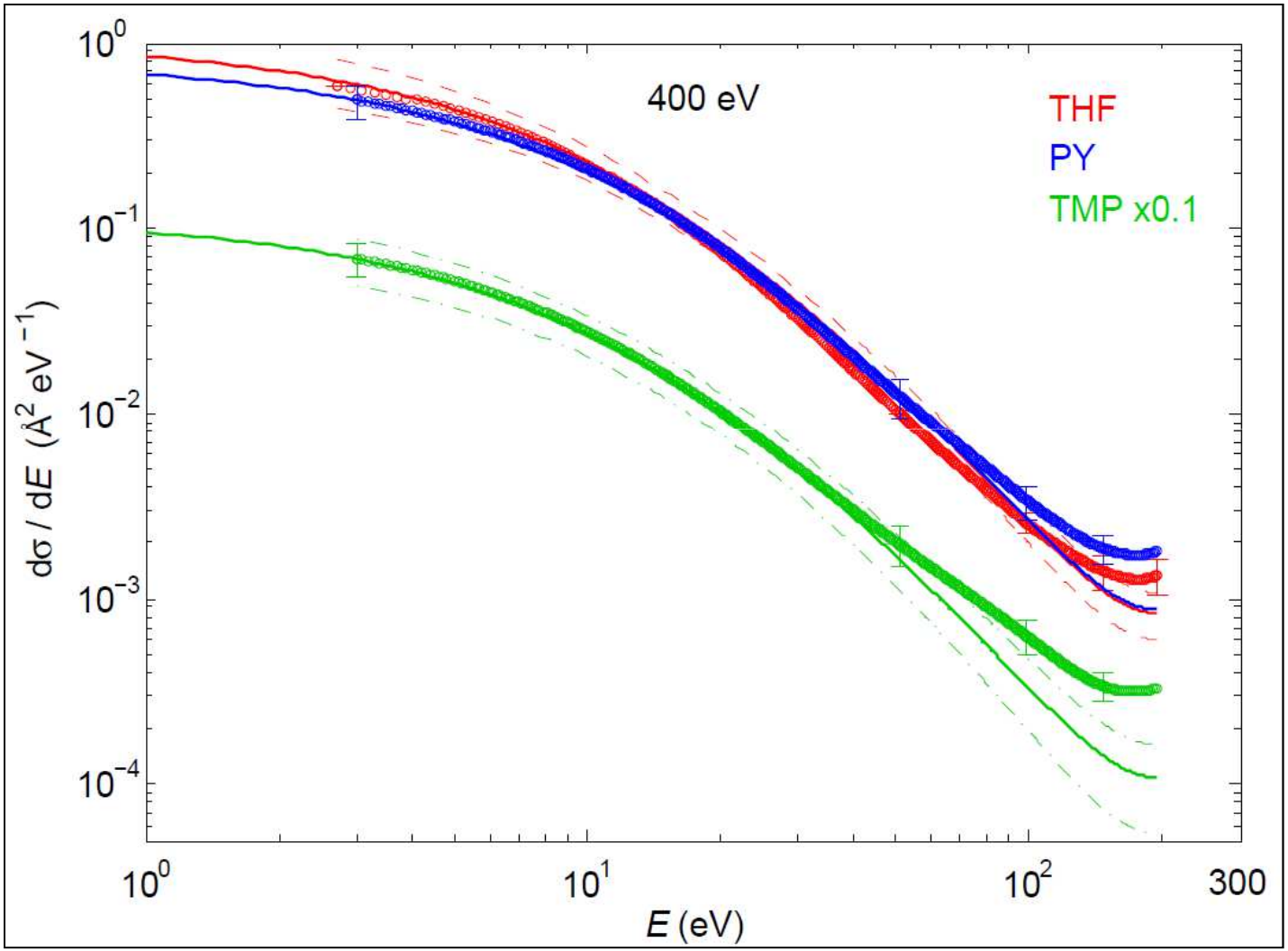
with $t' = T/P_2, \quad w' = E/P_2$

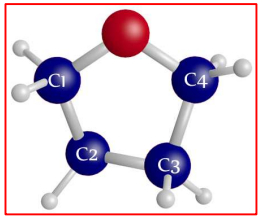
$$f_n(w) = (w+1)^{-n}, \quad f_n(t-w) = (t-w)^{-n}$$

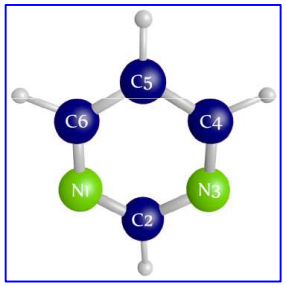
$$F_1 = -(t'+1)^{-1}, \quad F_2 = 1, \quad F_3 = P_4 \ln t'$$

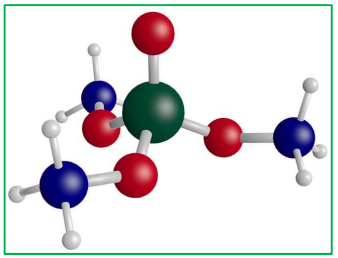
- Fit of parameters $P_{1\text{-}4}$ as a function of primary electron energy T

Single-differential ionisation CS









Data evaluation
Example: Ionisation-CS

PTB
CENTRE FOR MEDICAL RADIATION PHYSICS

Evaluation:

Experimental data as a function of T, E und Ω

↓

Fit of spline function as a function of E

↓

Fit of model function as a function of θ → $d^2\sigma_{ion}/dEd\Omega$

↓

Integration over $d\Omega$

↓

Fit of model function as a function of E → $d\sigma_{ion}/dE$

↓

Integration over dE

↓

Fit of model function as a function of T → σ_{ion} und $\sigma_{ion,i}$

Simulation:

Ionisation using σ_{ion}

y

Ionised molecular orbital, using $\sigma_{ion,i}$

↓

Secondary electron energy E, using $d\sigma_{ion}/dE$

↓

Polar scattering angle ϑ_s using $d^2\sigma_{ion}/dEd\Omega$

Total ionisation CS

- By integration $\sigma_{\text{ion}}(T) = \int_0^{(T-B_0)/2} \frac{\mathrm{d}\sigma_{\text{ion}}}{\mathrm{d}E}\,\mathrm{d}E$

- Binary-Encounter-Bethe model

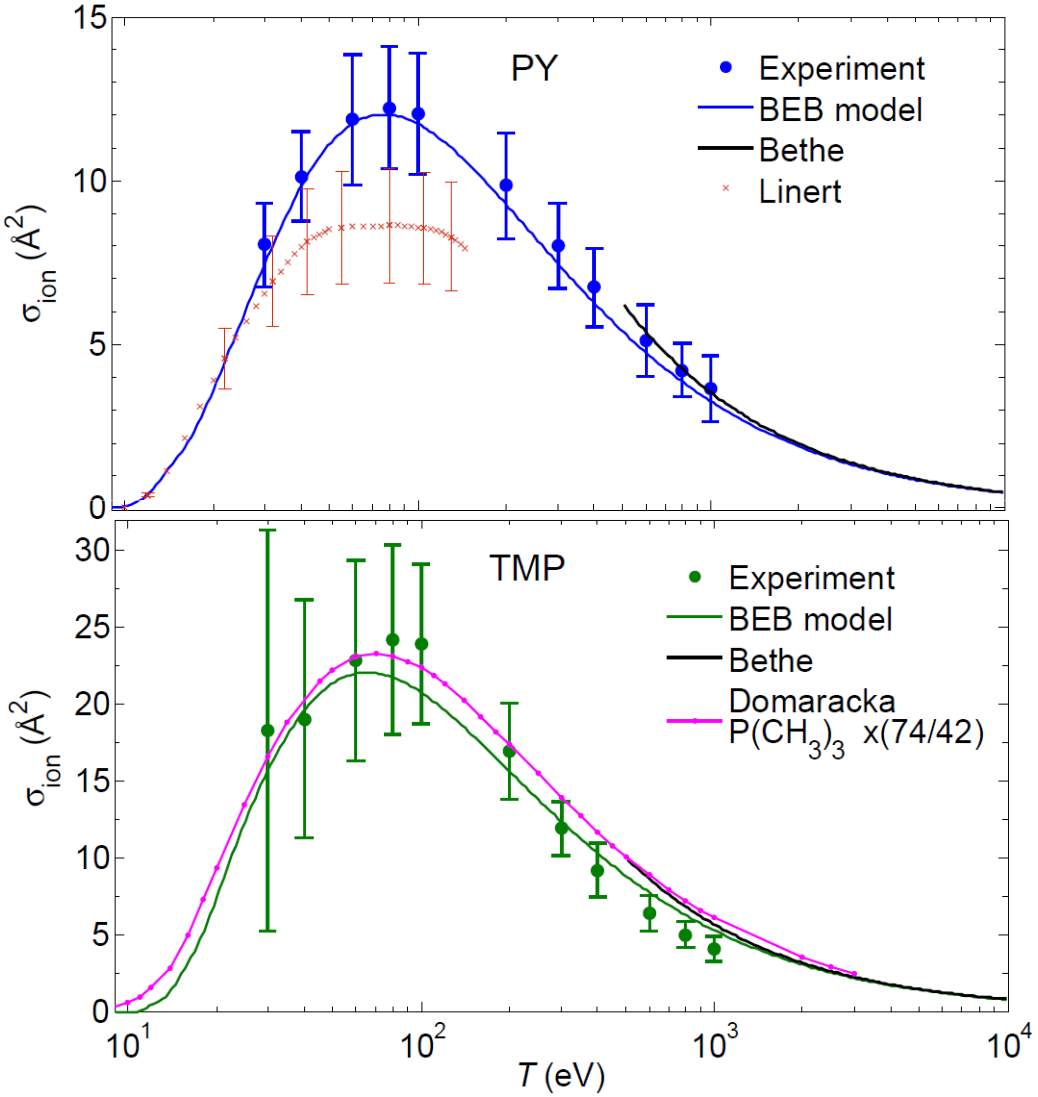
$$\sigma_{\text{ion}} = \sum_i \frac{4\pi\, a_0^2 N_i (R/B_i)}{t + (u+1)/n_i}\left[0.5\left(1-\frac{1}{t^2}\right)\ln t + 1 - \frac{1}{t} - \frac{\ln t}{t+1}\right]$$

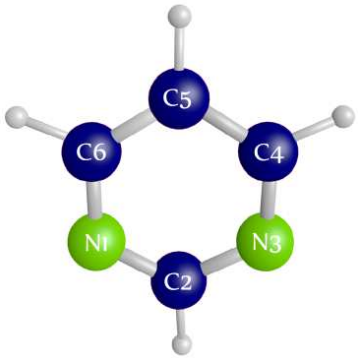
with

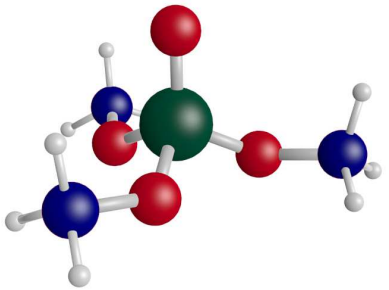
$t = T/B_i\,, \quad w = E/B_i\,, \quad u = U_i/B_i$

- Binding energies B_i and average kinetic energies U_i of molecular electrons calculated by GAMESS (the General Atomic and Molecular Electron Structure System, Gordon research group)

Total ionisation CS



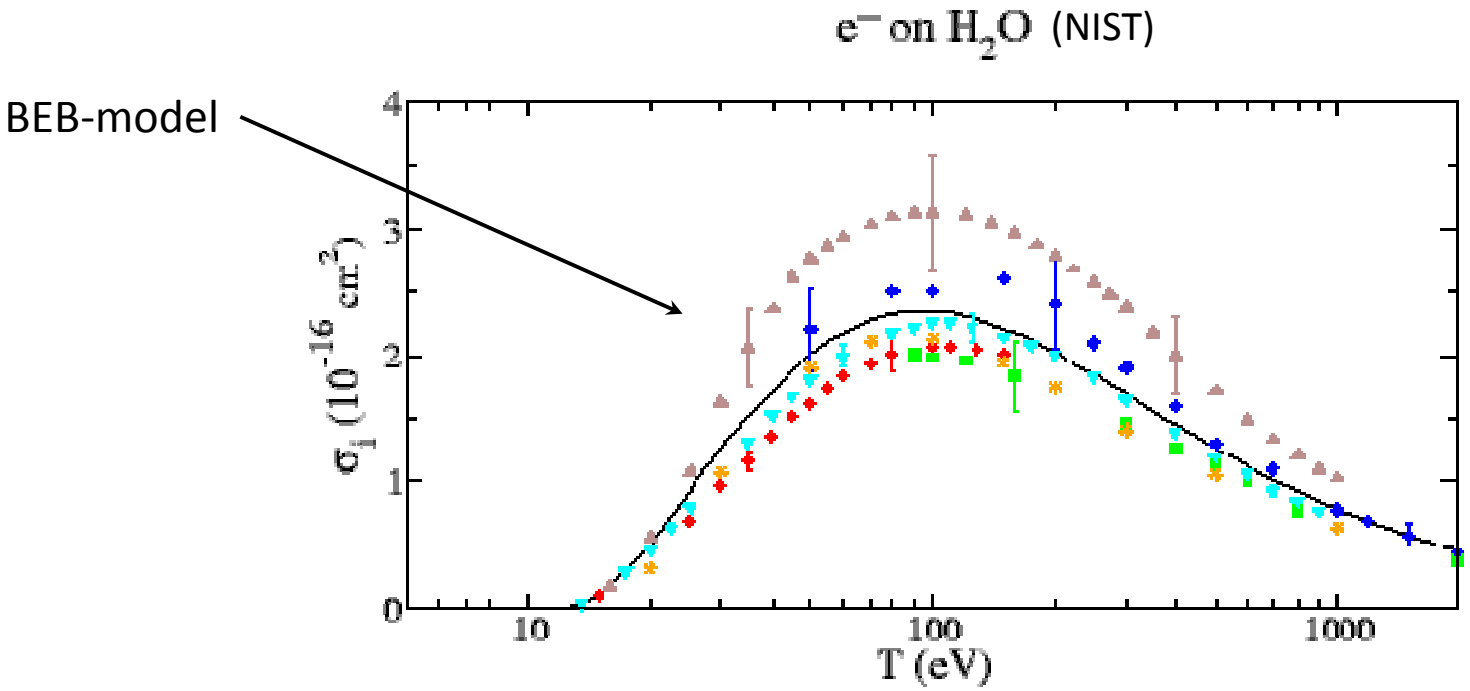




How different are cross sections (CS) of water and DNA constituents for electrons with energies 7 eV – 1 keV?

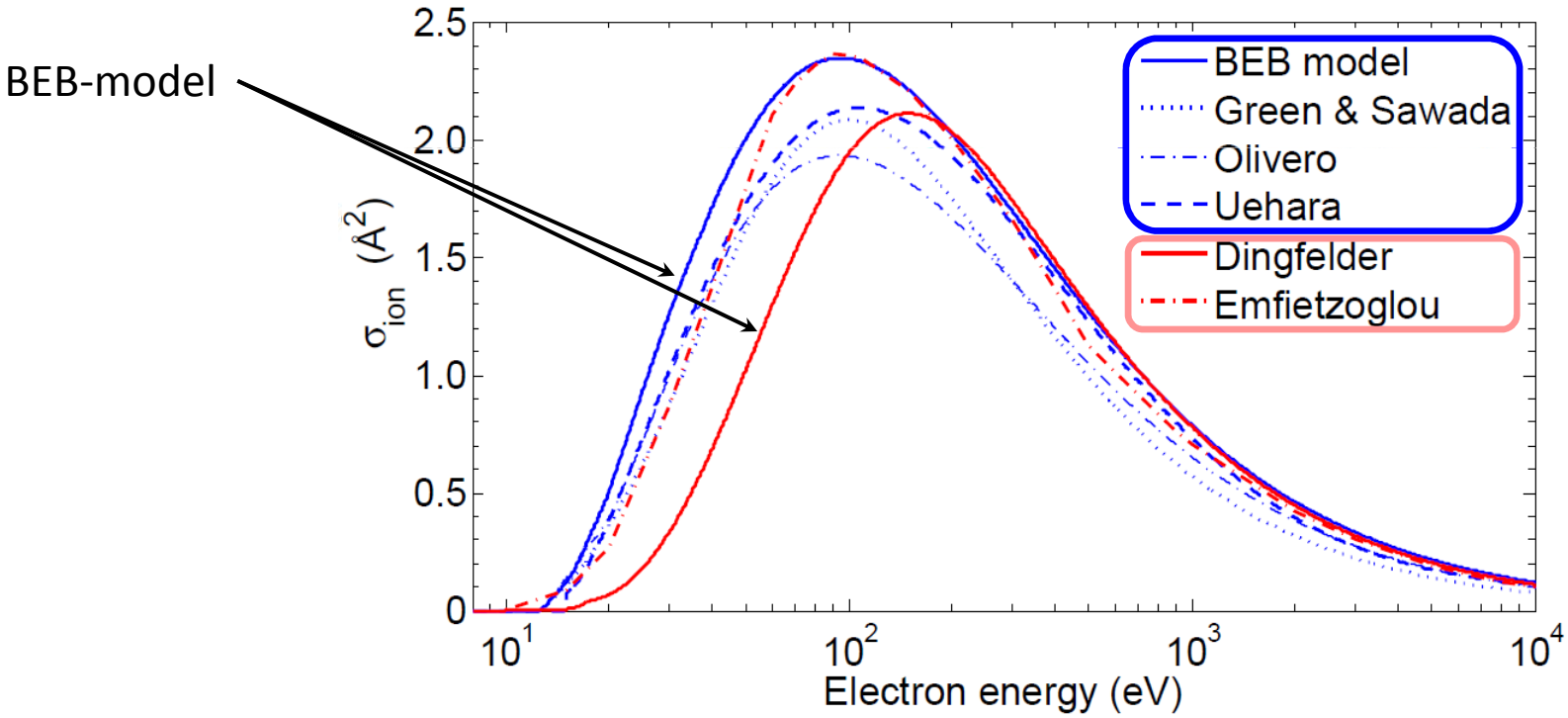
Electron CS of water

- Ionisation:
  - vapour: 1.25 – 2.0x

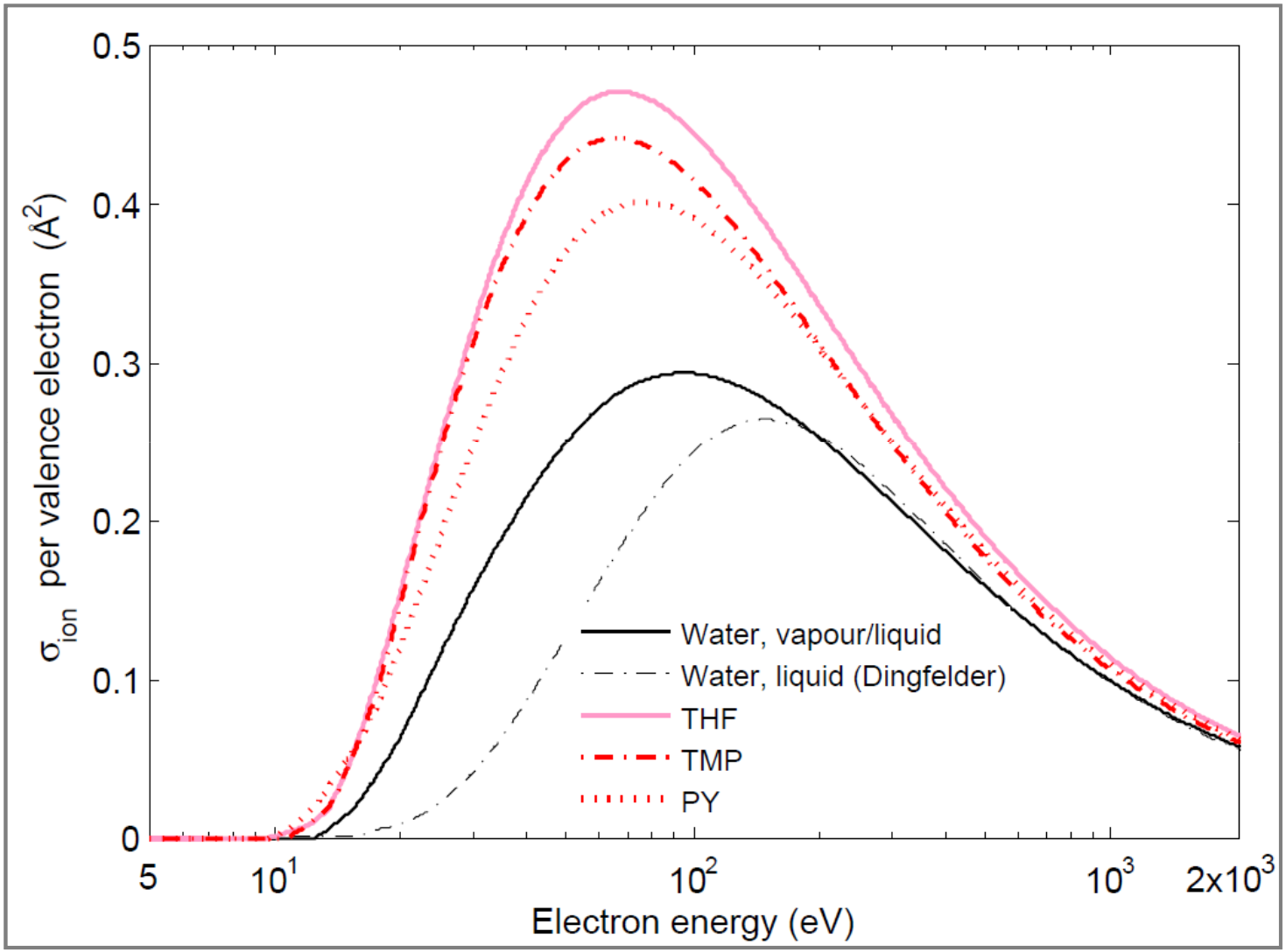


Electron CS of water

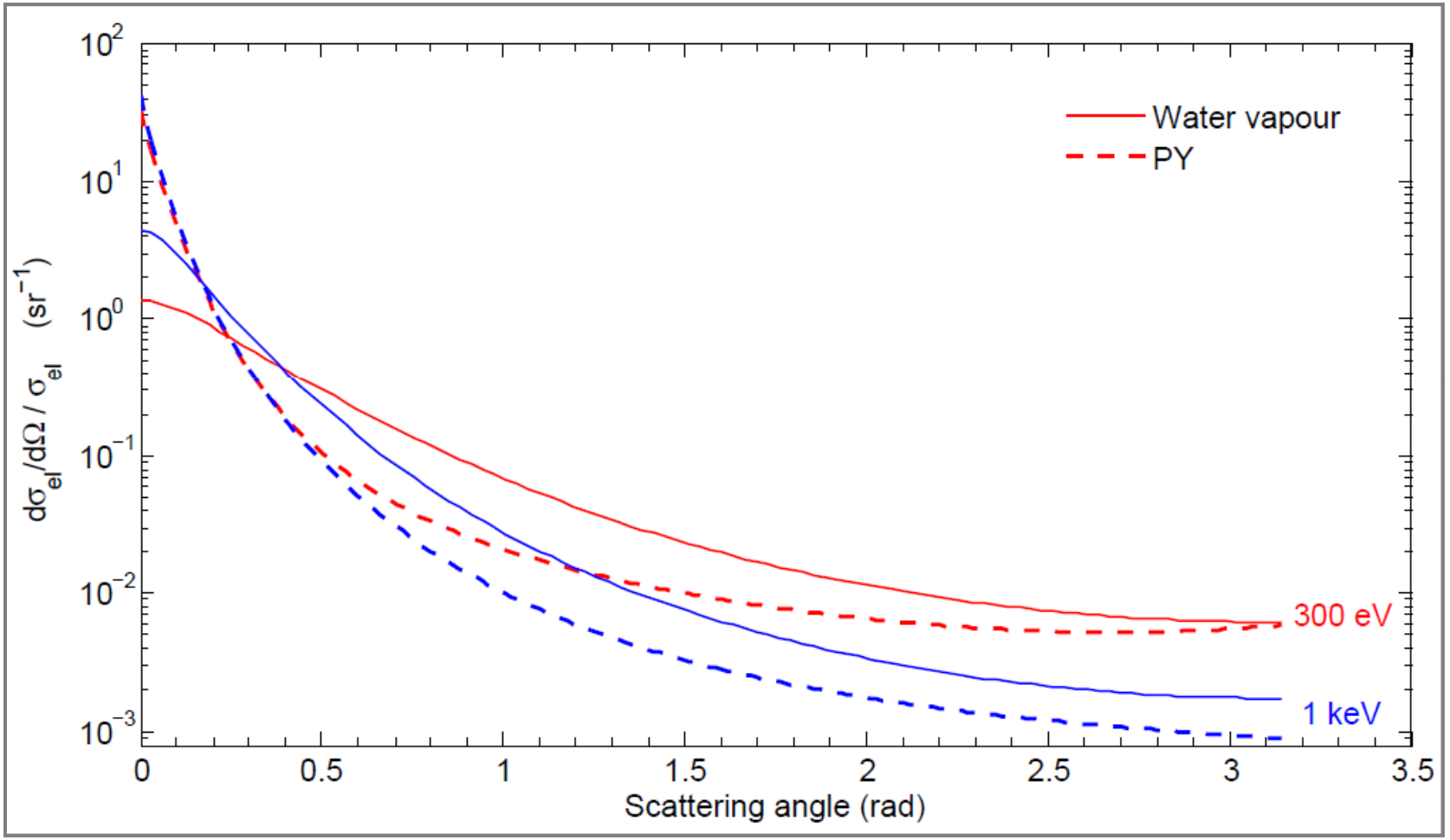
- Ionisation:
  - vapour: 1.25 – 2.0x
  - liquid: < 2x
- Excitation (electronic):
  - CS of water vapour 4x larger than of liquid water



Difference between CS of water and DNA molecules



Difference between CS of water and DNA molecules



How sensitive are simulated track structure parameters to differences in CS data?

‚DNA' medium

Homogeous distribution of congeneric nucleotides consisting of:

i.) Tetrahydrofuran and trimethylphosphate

ii.) Pyrimidine and purine

iii.) Water content in DNA depends on sequence of nucleobases;

≥ 8.0 H_2O / NT required for B-form M. Chaplin, Nat. Rev. 7, 861 (2006)

≥ 12.5 H_2O / NT within DNA helix M. Egli et al., Biopolymers 48, 234 (2000)

$$1/\lambda_{NT} = n_{NT}\left(\sigma_{THF} + \sigma_{TMP} + 0.5\left(\sigma_{PY} + \sigma_{PU}\right) + N_{H_2O}\,\sigma_{H_2O}\right)$$

$$n_{NT} = \frac{20}{\pi\, r_{10bp}^2\, h_{10bp}}$$

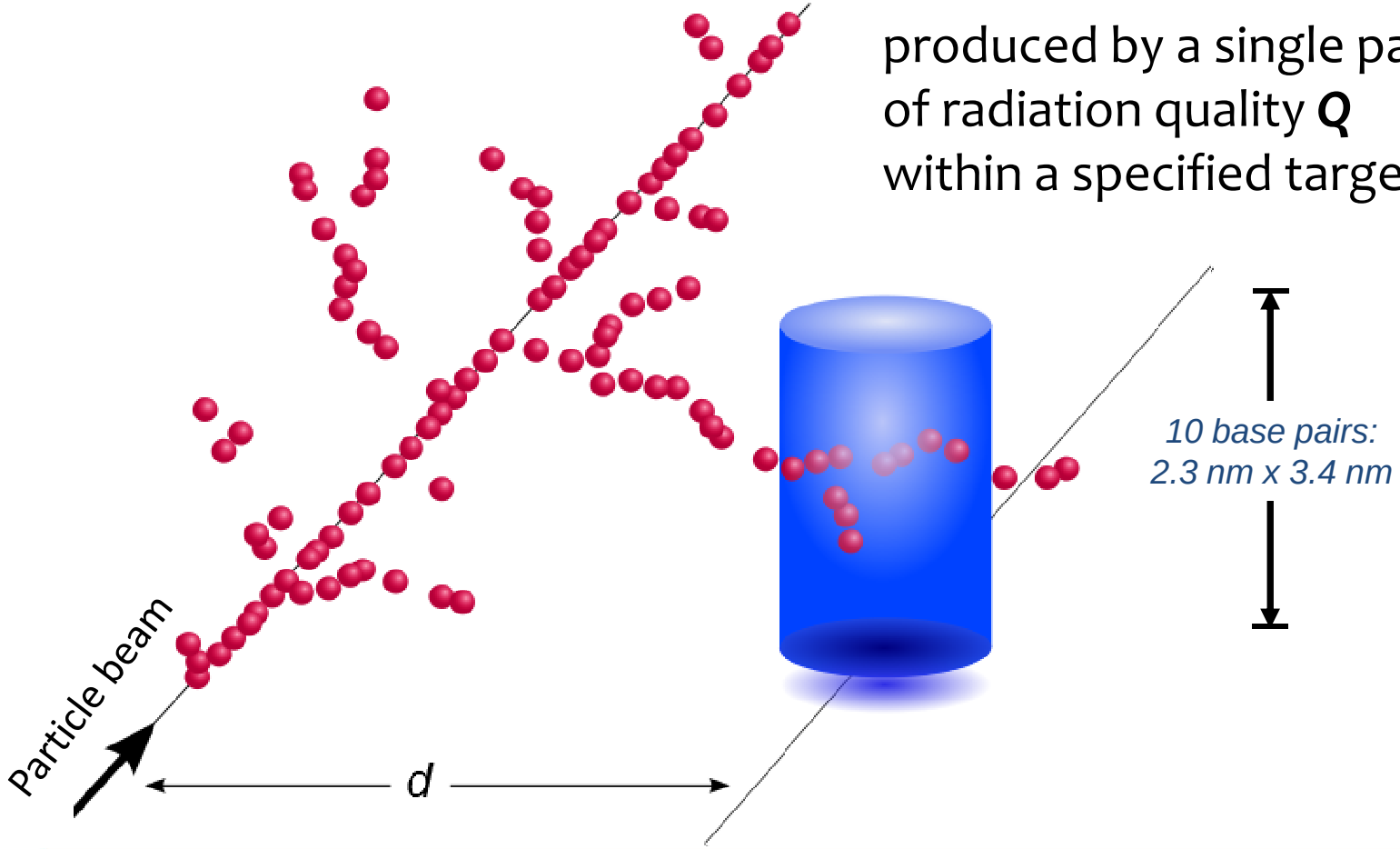
Comparison water/DNA with $\rho = 1\ g/cm^3$ $= M_{NT}\, n_{NT} / N_{Avogadro}$

N_{H_2O} = 6.28 H_2O/NT

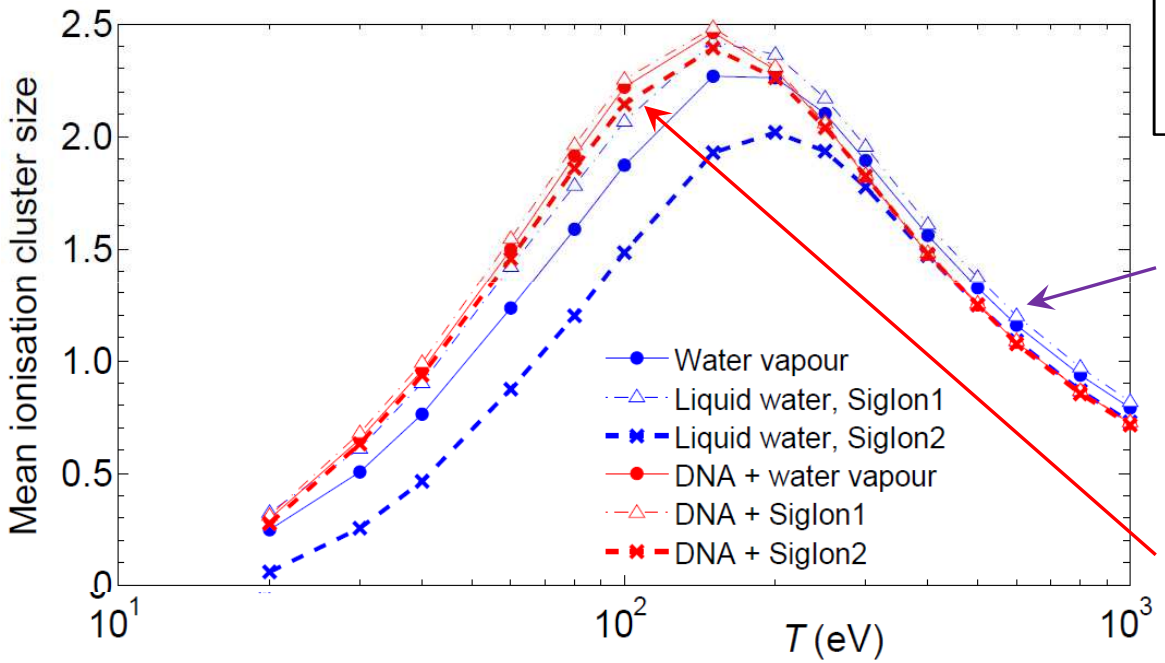
Characterisation of particle track structure

Ionisation cluster size:

Number of direct ionisations **ν** produced by a single particle of radiation quality **Q** within a specified target volume



Simulated track structure parameters of electrons in water and DNA medium

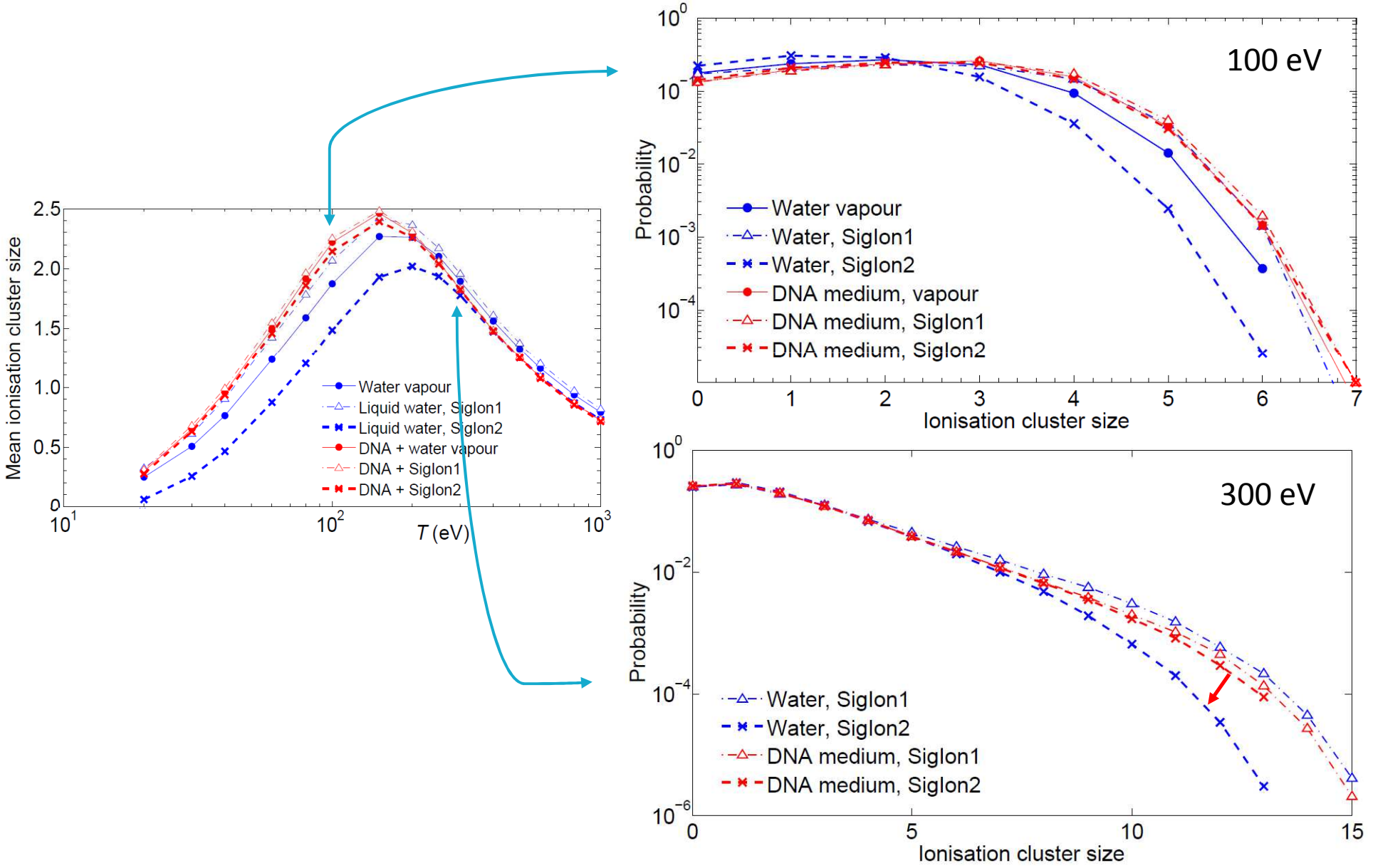


Different ionisation CS of water:
SigIon1: σ_{ion} Emfietzoglou
SigIon2: σ_{ion} Dingfelder

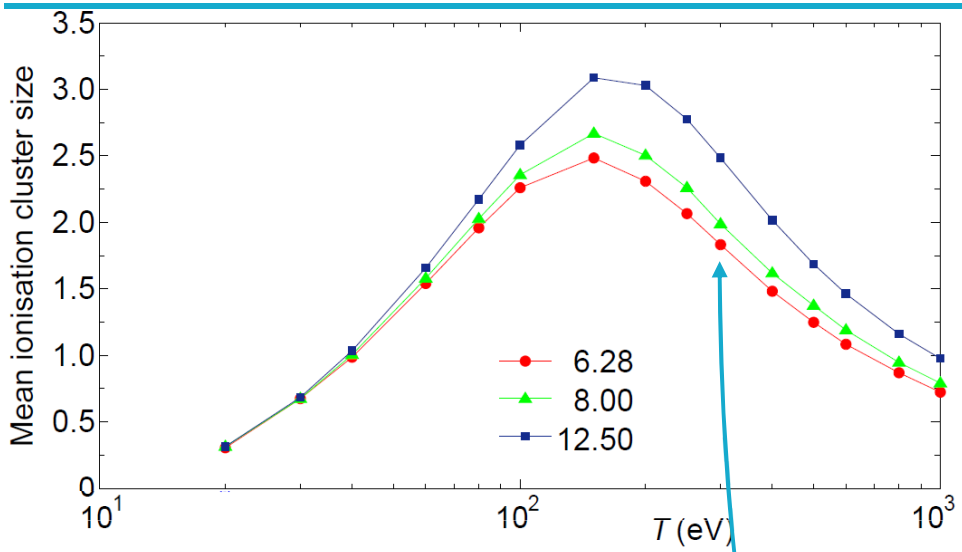
DNA vs. Wasser:
- up to 12% difference to SigIon1
- SigIon2 25% lower in maximum
  2x lower at 40 eV

Different CS of water used in DNA-Medium:
- up to 11% variation

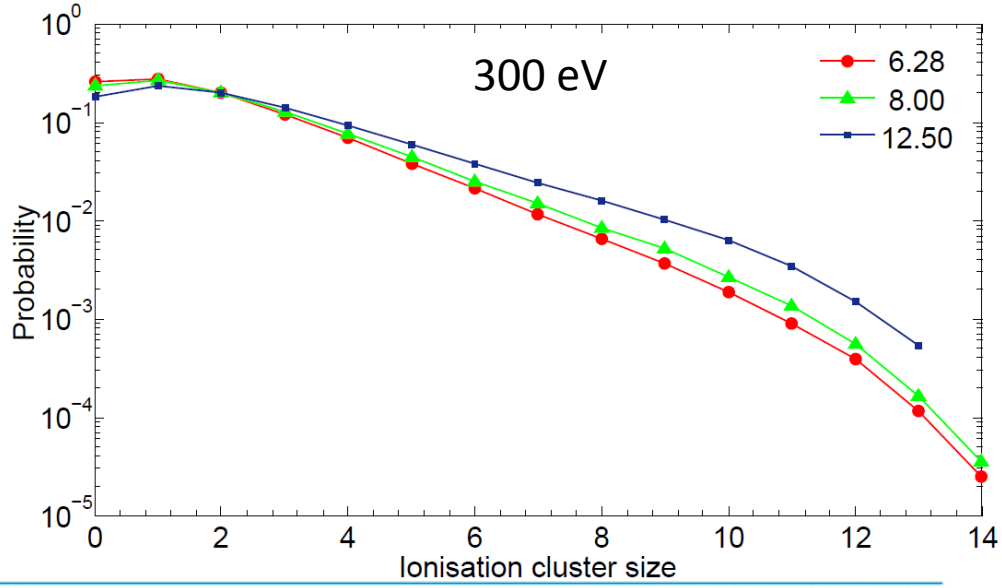
Ionisation cluster size distributions



Influence of water content in DNA medium



Realistic water content:
25-35% larger mean cluster size



Summary

PTB
CENTRE FOR MEDICAL RADIATION PHYSICS

- How different are electron-impact CS of water and DNA constituents?
  - Significant differences in
    - energy dependence of total CS and
    - angular dependence of differential CS

- How sensitive are simulated track structure parameters to differences in CS data?
  - Results in DNA medium of same mass density similar to those in liquid water using Emfietzoglou‘s ionisation CS
  - Realistic water content of DNA medium leads to significantly enhanced probabilities to produce large ionisation clusters

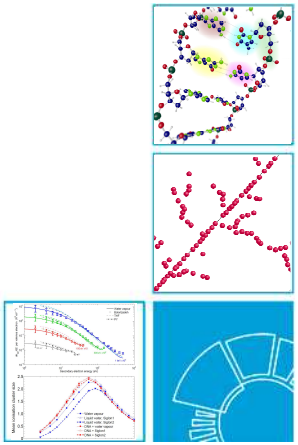
ACKNOWLEDGEMENT

Hans Rabus, Woon Yong Baek, Gerhard Hilgers, Heidi Nettelbeck, Daniel Bennett
Physikalisch-Technische Bundesanstalt (PTB), Germany

Anatoly Rosenfeld, Susanna Guatelli
Centre for Medical Radiation Physics (CMRP), Australia

Elisabetta Gargioni
University Medical Center Hamburg-Eppendorf (UKE), Germany

The work reported here was carried out within the EMRP Joint Research Project SIB06 BioQuaRT. The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union.



Physikalisch-Technische Bundesanstalt
Braunschweig und Berlin
Bundesallee 100
38116 Braunschweig

Marion Bug
Department 6.6 Fundamentals of Dosimetry

Phone: +49 (0)531 592-6631
E-mail: marion.bug@ptb.de
www.ptb.de

Status: 05/14