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PROTON TRACK-STRUCTURE IN BIOLOGICAL MATTER: WATER vs DNA

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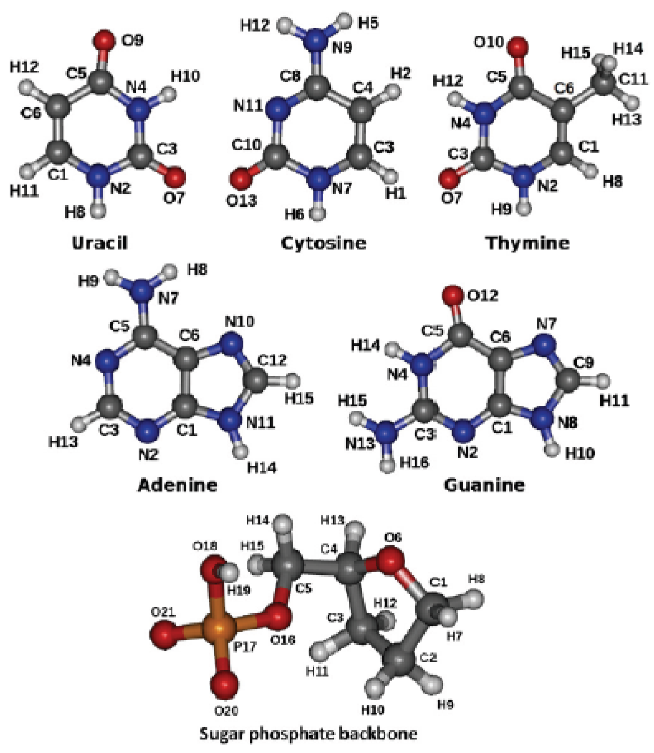
Understanding the radio-induced biological effects like **cellular death** and **chromosomal aberrations** need the knowledge of the underlying physics of the irradiation.
Total and multi-differential cross sections relative to the ionizing processes induced by heavy charged particles along their track represent useful input data for **numerical track-structure simulations**.

In this context, we have recently provided a series of theoretical works dedicated to the description of the **proton-induced ionization and capture processes on DNA components** (nucleobases and sugar-phosphate backbone).

In the current work, the biological targets are described via their molecular orbitals by employing the quantum chemical **GAUSSIAN 09 program**.

The target wave functions are computed at the **Hartree-Fock level** optimized at the MP2/6-31G(d) computational level, *i.e.* by including **correlation calculations** at the second order of perturbation theory MP2 and by using GAUSSIAN-type orbitals added to a double-zeta valence shell and polarization orbitals on non-hydrogen atoms.

The ionization potentials (IP's) calculated at the RHF/3-21G level **are in good agreement with the experiments**.



Two quantum-mechanical approaches for modelling the ionization process

1st Born approximation (CB1-CW)

$$\varphi_\alpha^+ = \frac{\exp(i\boldsymbol{K}_\alpha.\boldsymbol{R})}{(2\pi)^{3/2}}\phi_\alpha(\boldsymbol{x})\exp\left[-i\frac{Z_P}{v}\ln(vR - \boldsymbol{v}.\boldsymbol{R})\right]$$

effective charge

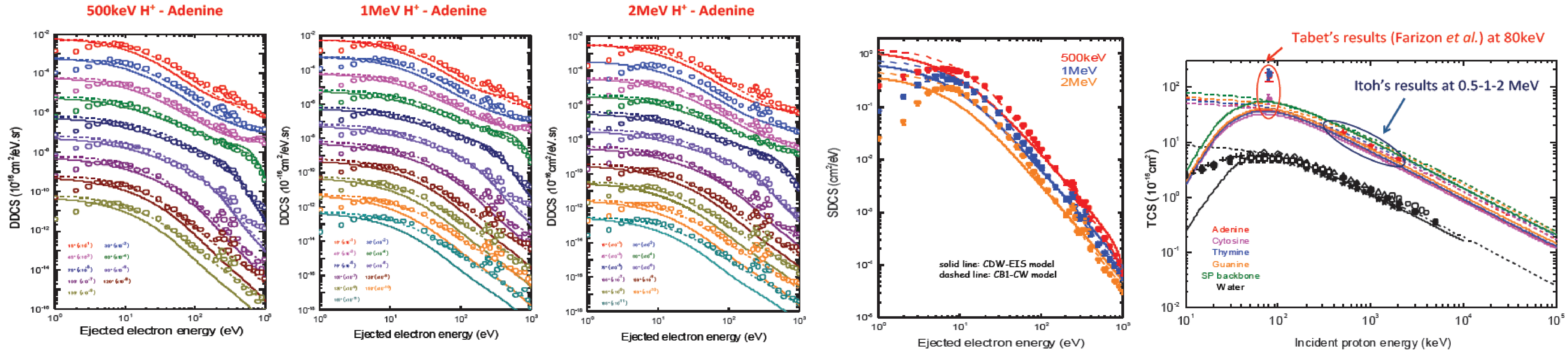
$$Z_T^* = \sqrt{-2n_\alpha^2\varepsilon_\alpha}$$

$$\varphi_\beta^- = \frac{\exp(i\boldsymbol{K}_\beta.\boldsymbol{R})}{(2\pi)^{3/2}}\phi_\beta(\boldsymbol{x})N^*(Z_T^*/k)\,{}_1F_1(-iZ_T^*/k;1;-ikx - i\boldsymbol{k}.\boldsymbol{x})\times\exp\left[+i\frac{Z_P}{v}\ln(vR + \boldsymbol{v}.\boldsymbol{R})\right]$$

Continuum Distorted Wave – Eikonal Initial State (CDW-EIS)

$$\chi_\alpha^+ = \frac{\exp(i\boldsymbol{K}_\alpha.\boldsymbol{R})}{(2\pi)^{3/2}}\phi_\alpha(\boldsymbol{x})\exp\left[-i\frac{Z_P}{v}\ln(vs + \boldsymbol{v}.\boldsymbol{s})\right]$$

$$\chi_\beta^- = \frac{\exp(i\boldsymbol{K}_\beta.\boldsymbol{R})}{(2\pi)^{3/2}}\phi_\beta(\boldsymbol{x})N^*(Z_T^*/k)\,{}_1F_1(-iZ_T^*/k;1;-ikx - i\boldsymbol{k}.\boldsymbol{x})\times N^*(Z_P/p)\,{}_1F_1(-iZ_P/p;1;-ips - i\boldsymbol{p}.\boldsymbol{s}),$$



References

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Galassi *et al.*, *Phys. Med. Biol.* **57**, 2081 (2012); Champion *et al.*, *Phys. Med. Biol.* **57**, 3039 (2012); Itoh *et al.*, *Phys. Rev. A* **88**, 052711 (2013).

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