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New Geant4-DNA physics model for simulating gold nanoparticle radio-enhancement: Benchmarking calculations of cross sections and stopping power from 10eV to 1MeV

I. Polopetrakis[1], I. Kyriakou[1], D. Sakata[2], S. Incerti[3], S. Guatelli[4], P. Karaiskos[5], D. Emfietzoglou[1]

[1]*Medical Physics Laboratory, Department of Medicine, University of Ioannina, Ioannina, Greece*

[2]*Division of Health Sciences, Osaka University, Osaka, Japan*

[3]*Univ. Bordeaux, CNRS, LP2I, Gradignan, France*

[4]*Center of Medical Radiation Physics, University of Wollongong, Wollongong, Australia*

[5]*Medical Physics Laboratory, Medical School, National and Kapodistrian University of Athens, Athens, Greece*

1. Background-Aim

- Gold nanoparticles (GNPs) are currently being studied as a means to increase therapeutic efficacy in radiotherapy by increasing the local dose in the closest vicinity around the GNP, due to the emission of low-energy Auger and Photoelectrons

- Conventional Monte Carlo dosimetry codes are ill-suited, as they offer limited resolution (~mm) and are reliable for energies well-above 1 keV

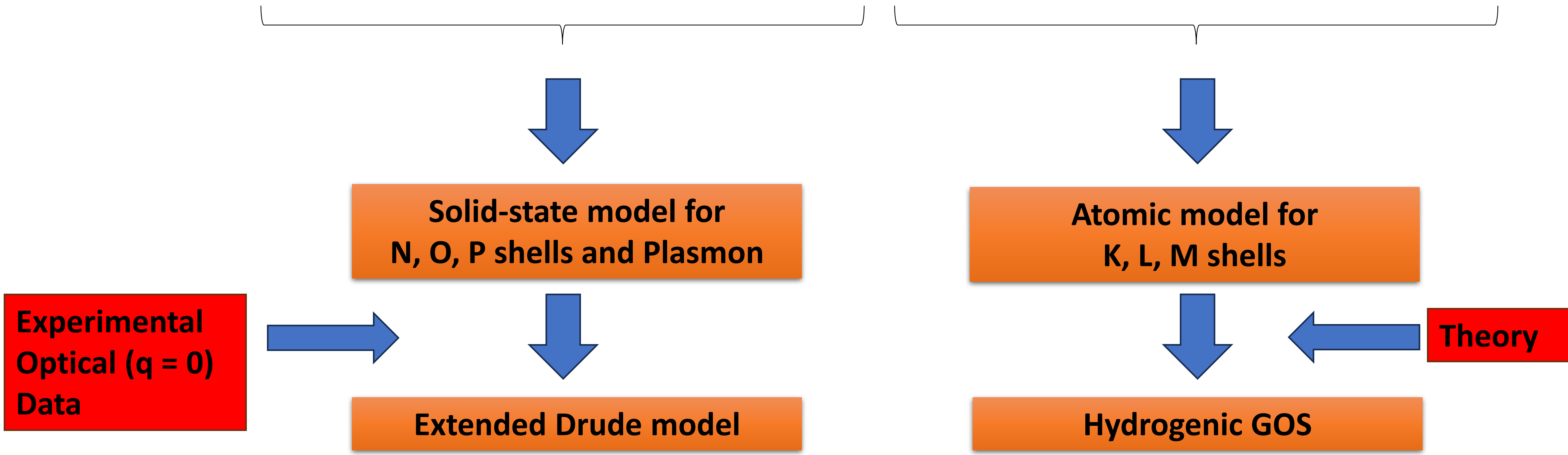
- Discrete physics ("Track-Structure") models are necessary for studying the energy deposition at the nanoscale by these low-energy (sub-keV) electrons

Improvements to the Geant4-DNA Energy-Loss model for Gold:

- The Energy-Loss channels (Ionizations, Excitations, Plasmon) are treated by the Dielectric Theory rather than different theories
  - ✓ Ensures self-consistency and Robustness
  - ✓ Accounts for condensed-phase effects
  - ✓ Based on experimental data for Au
  - ✓ Much more accurate calculations of Cross-Section and Stopping Power down to 10eV

Energy-Loss Function (ELF) for Au

$$Im\left[\frac{-1}{\varepsilon(w,q)}\right]_{Total} = \sum_j^{Outer+Plasmon} \frac{A_j \gamma_j w}{\left(w^2 - E_j^2(q)\right)^2 + (w\gamma_j)^2}\,\Theta(w - B_j) + 8\pi^2 a_0^3 Ry^2 N \sum_j^{Inner} \frac{1}{w}\frac{df(w,q)}{dw}\,\Theta(w - B_j)$$



Relativistic Plane Wave Born Approximation (RPWBA)

The DCS for each sub-shell is the Sum of a Longitudinal (L) and a purely relativistic Transverse (T) term

$$\frac{d\sigma^L_{Born}(w,T)}{dw} = \frac{1}{\pi a_0 N m c^2 \beta(T)^2} \int_{q_{min}}^{q_{max}} \frac{1}{Q(q)} \left(\frac{c^2 q}{\sqrt{c^2 q^2 + m^2 c^4}}\right)\left(\frac{1 + Q(q)/mc^2}{1 + Q(q)/2mc^2}\right) Im\left[\frac{-1}{\varepsilon(w,q)}\right] dq$$

Momentum-depended ELF

$$\frac{d\sigma^T_{Born}(w,T)}{dw} = \frac{1}{\pi a_0 N m c^2 \beta(T)^2}\left[ln\left(\frac{1}{1-\beta(T)^2}\right) - \beta(T)^2\right] Im\left[\frac{-1}{\varepsilon(w,q=0)}\right]$$

ELF at the Optical Limit

$$q_{min,max} = \frac{1}{c}\left(\sqrt{T(T+2mc^2)} \mp \sqrt{(T-w)(T-w+2mc^2)}\right)$$

$$Q(q) = c\sqrt{q^2 + m^2c^2} - mc^2$$

Energy corrections beyond the First-Born Approximation

- Exchange (EX) and "Coulomb-field" (CO) corrections are included in the Longitudinal term of the DCS and account for spin and short range Coulomb interactions respectively

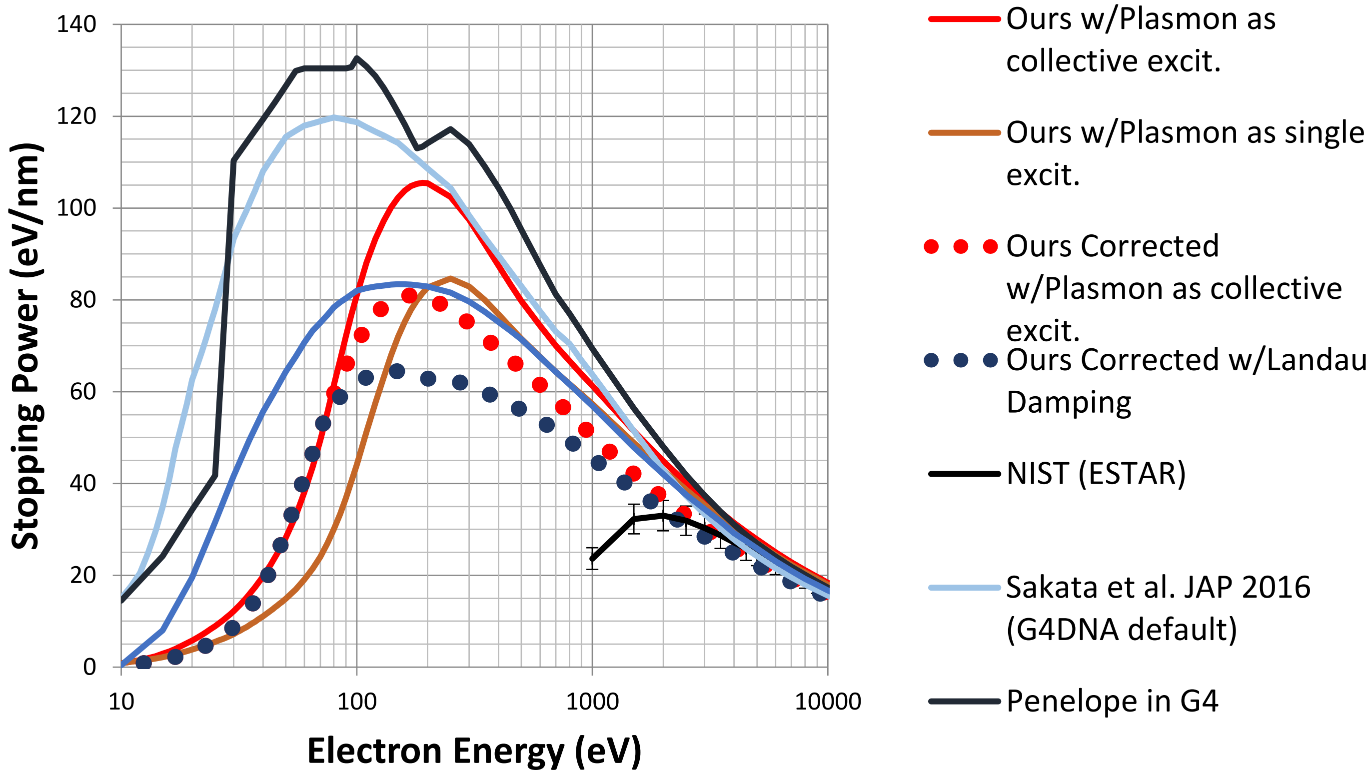
$$DCS^L_{Born-EX-CO}(w,T) = DCS^L_{Born}(w,T+B_j+U_j) + DCS^L_{Born}(T+2B_j+U_j-w,T+B_j+U_j) - \sqrt{DCS^L_{Born}(w,T+B_j+U_j) * DCS^L_{Born}(T+2B_j+U_j-w,T+B_j+U_j)}, \text{ for Ionizations}$$

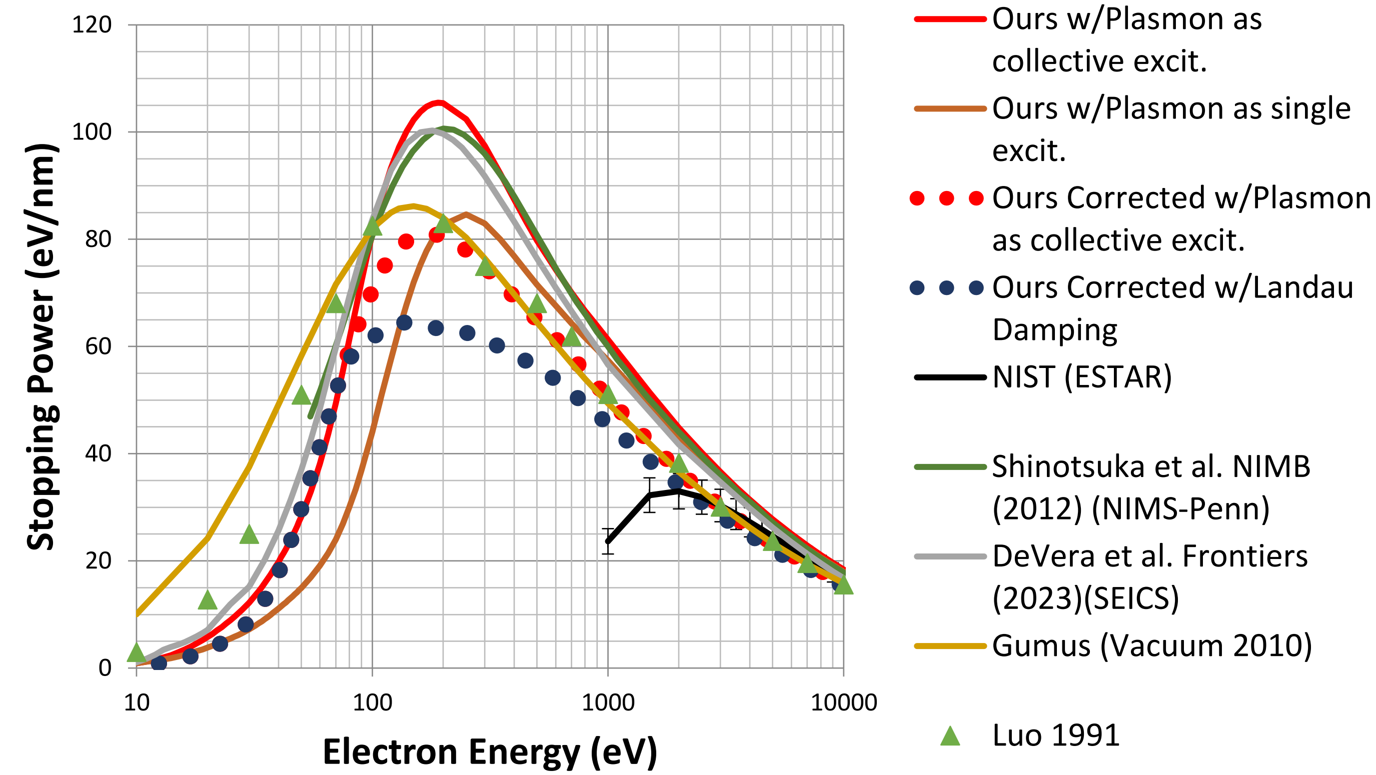
$$DCS^L_{Born-CO}(w,T) = DCS^L_{Born}(w,T+2E_j), \text{ for Excitations}$$

- **Based on the Landau Mechanism, there is a critical value of energy-transfer (w_c), above which the plasmon can decay by transferring all its energy into a single electron, which can then undergo an ionization**

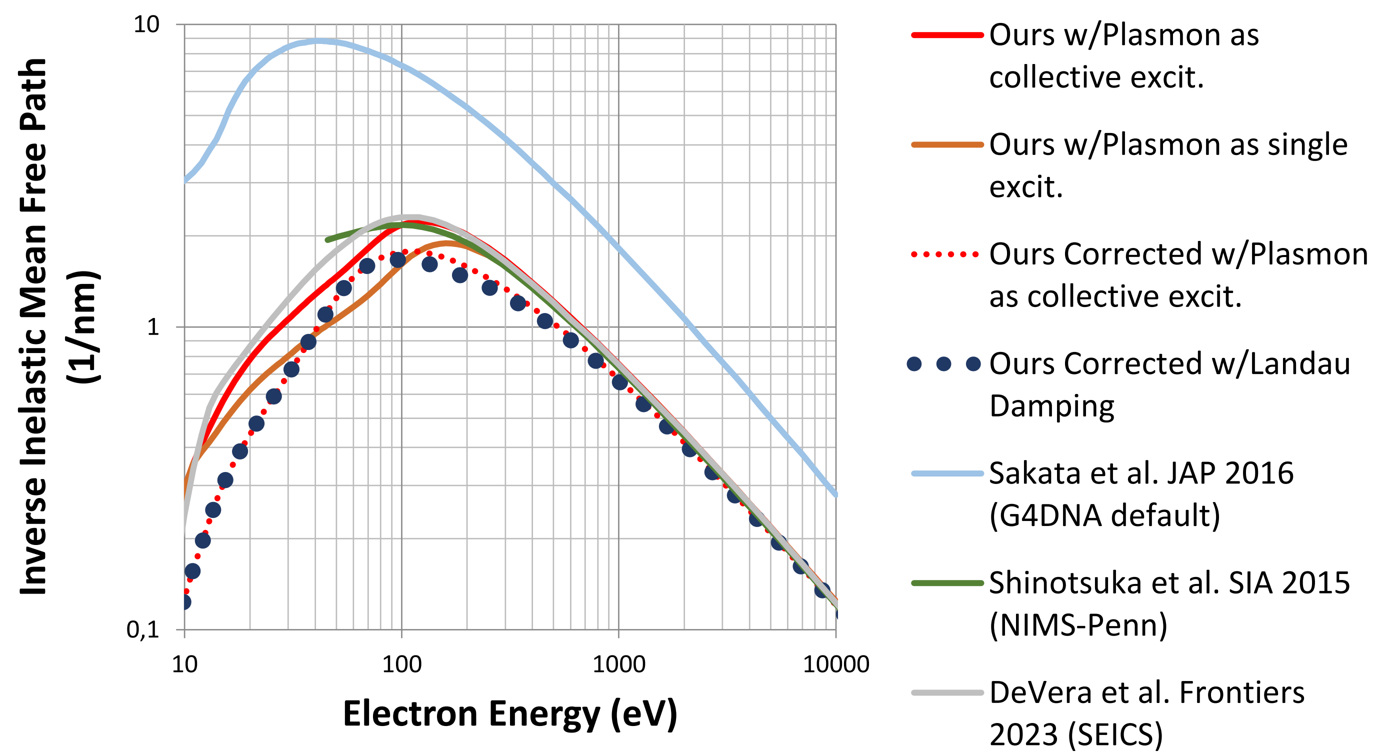
$$DCS^L_{Born-EX-CO}(w,T) = DCS^L_{Born}(w,T+2E_j) + DCS^L_{Born}(T+2E_j-w,T+2E_j) - \sqrt{DCS^L_{Born}(w,T+2E_j) * DCS^L_{Born}(T+2E_j-w,T+2E_j)}, \text{ for plasmon Ionization}$$

3. Results (1)



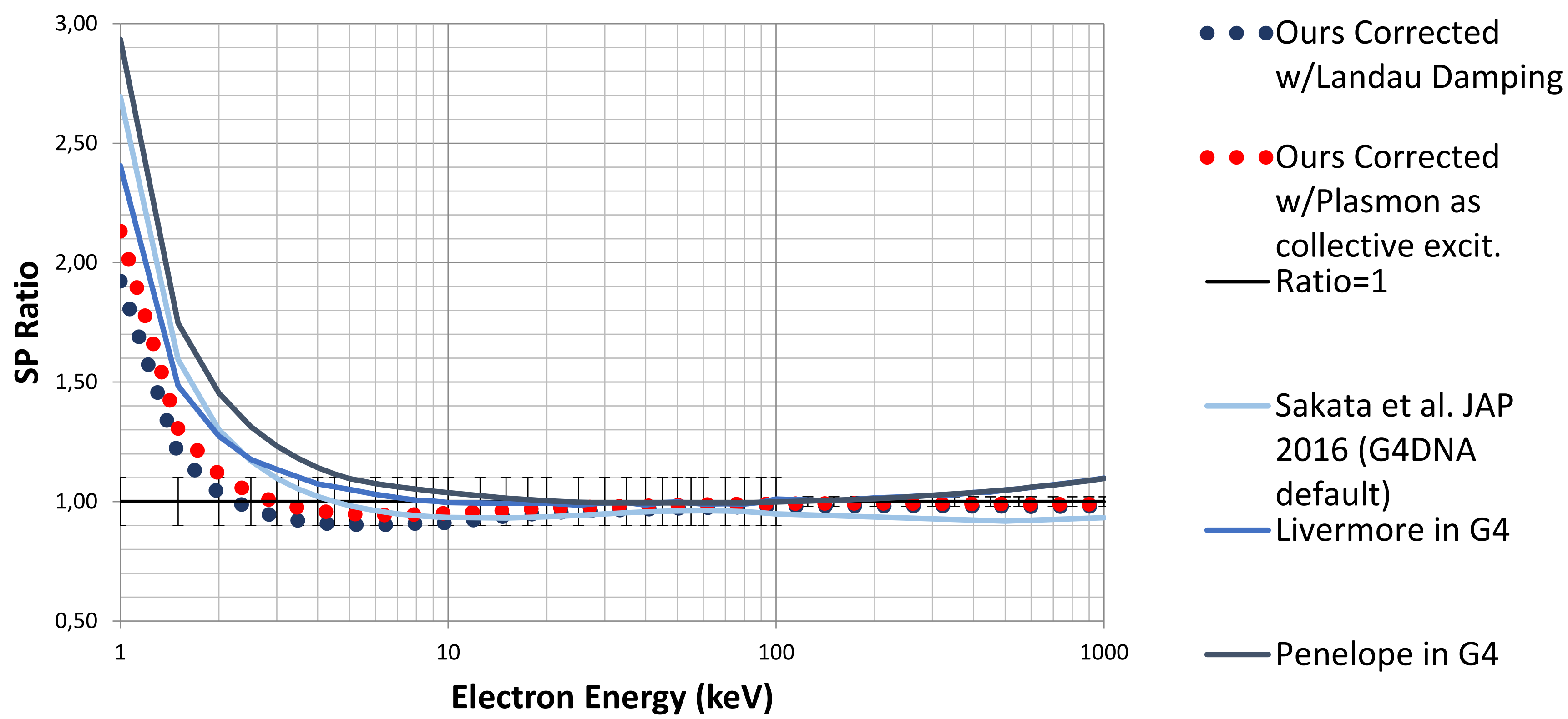


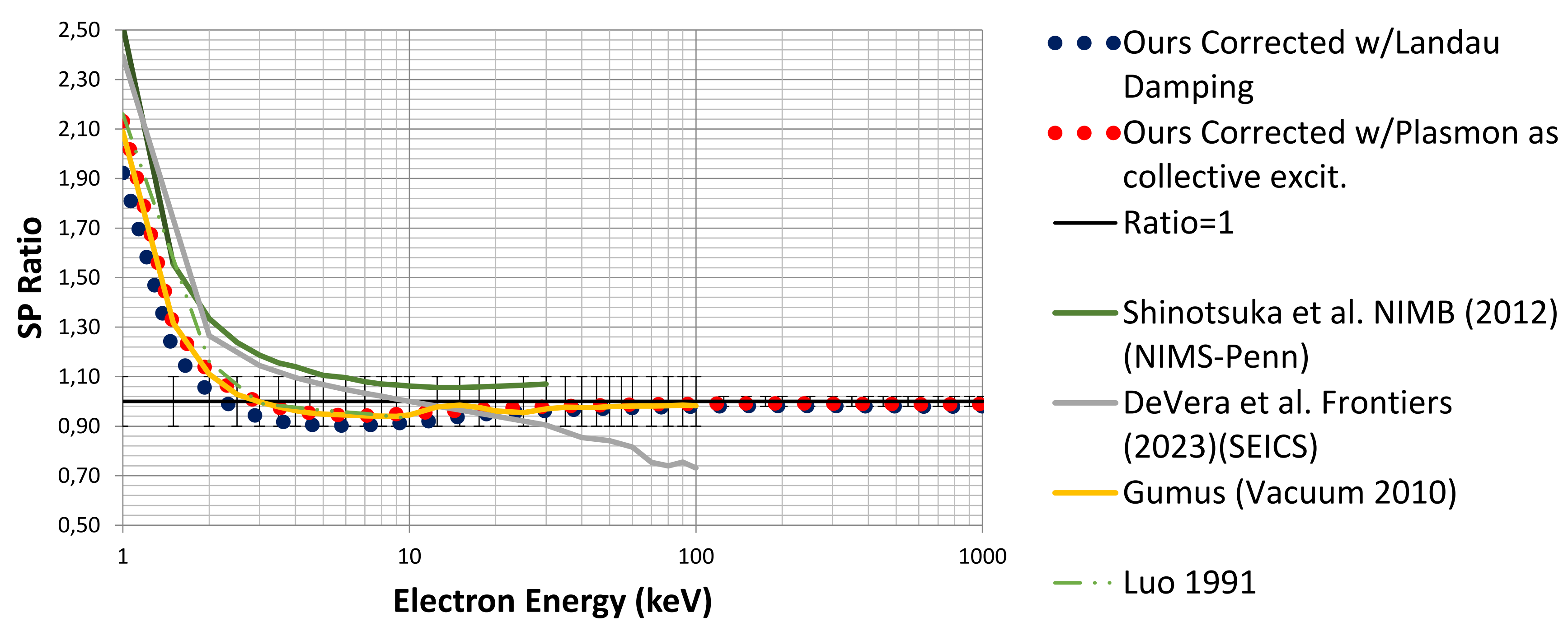
Major differences between models in the sub-keV range!



Landau Mechanism significantly decreases the SP (up to 40%)!

3. Results (2)





When NIST is used as reference, our models are within 10% up to 100keV and 2% up to 1MeV!

4. Conclusions

- A new Geant4-DNA cross section database for electron-GNP interactions that extends down to very low energies is under development
- Results reveal significant differences in the important energy range below ~1 keV due to the effects of exchange-correlation, dielectric screening, and plasmon decay
- The above effects are either neglected or not included fully (or consistently) in other studies
- The already existing Geant4 models clearly overestimate the Stopping Power and Cross-Section in the sub-keV energy range
- The new model is self-consistent and robust
- Hopefully it will be integrated in the Geant4-DNA-Au package for electron interactions with Gold

5. References

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6. Acknowledgements

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