Monte Carlo simulation of the transport of energetic electrons in materials of technological and biomedical interest

Ana María Zamora-Vinaroz, Mario Mompean-Herrero, Pablo de Vera, Rafael Garcia-Molina

Departamento de Física - Centro de Investigación en Óptica y Nanofísica

UNIVERSIDAD DE MURCIA

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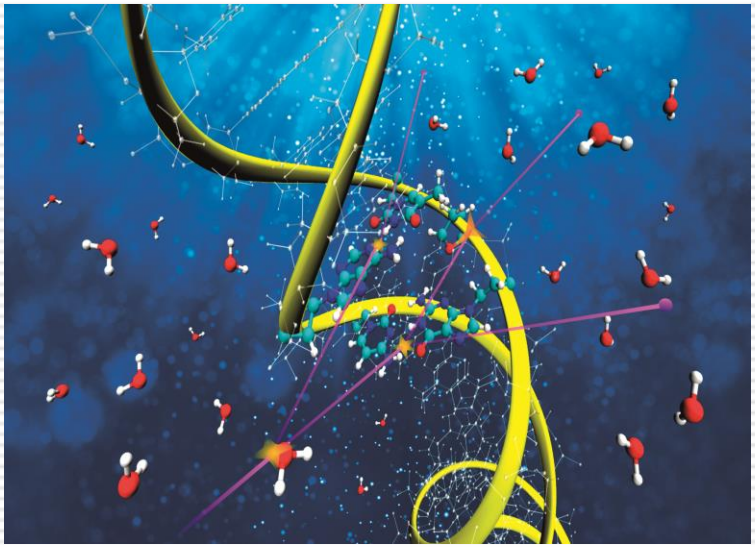
Energetic electrons

- Energy range: [~eV, ~MeV]
- Ubiquitous particles:

  Charged beams

  – Ionisation



P. de Vera, I. Abril, R. Garcia-Molina, *Phys. Chem. Chem. Phys.* **23** (2021) 5079-5095

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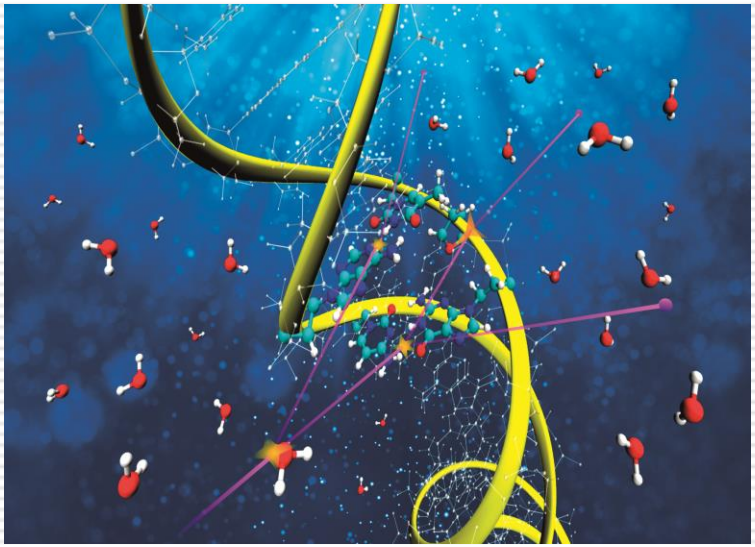

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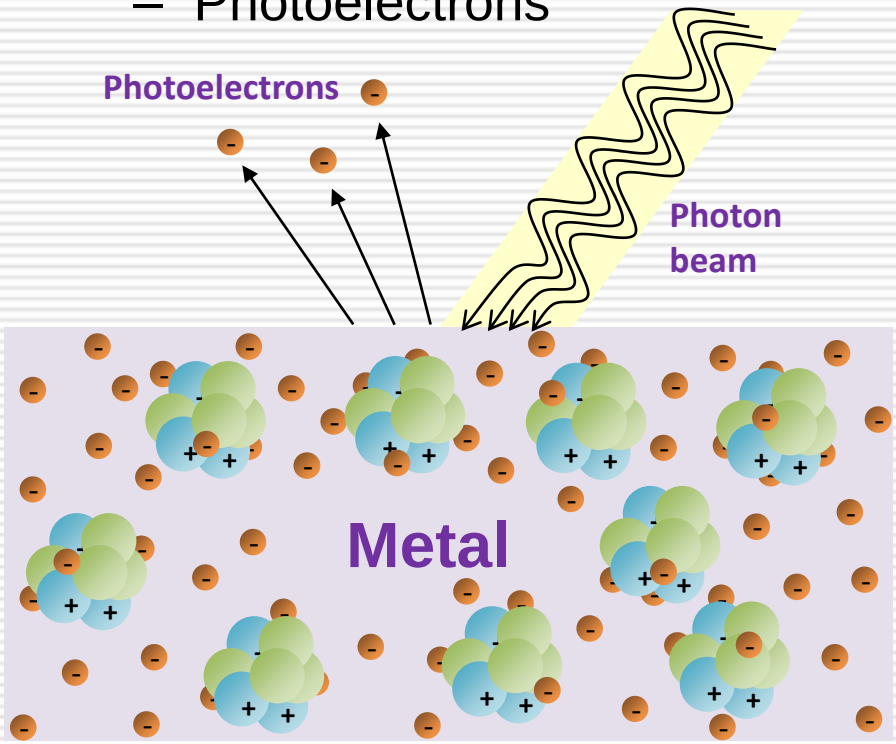
Photons

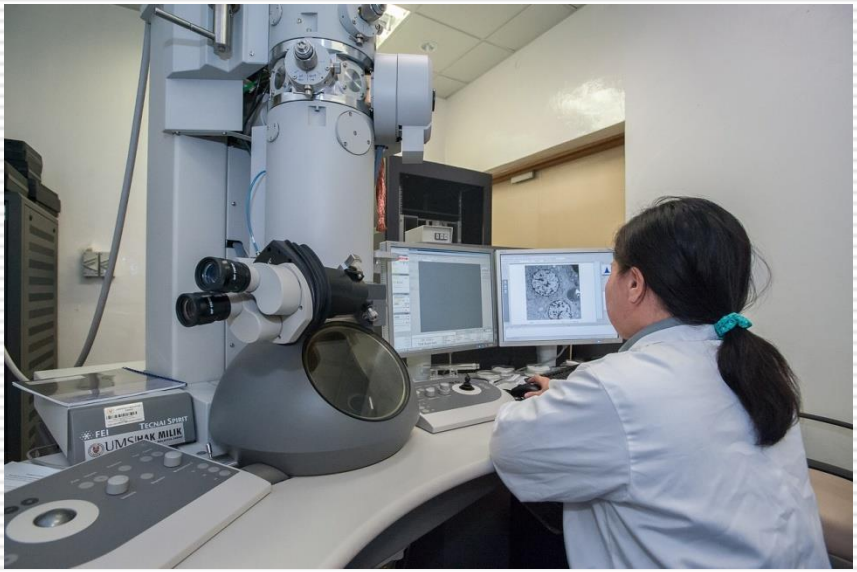
– Compton effect

– Photoelectrons



Applications of energetic electrons

Technological:
electron microscopy,
material surface analysis



W. S. M. Werner, *Surf. Interface Anal.* **31** (2001) 141-176

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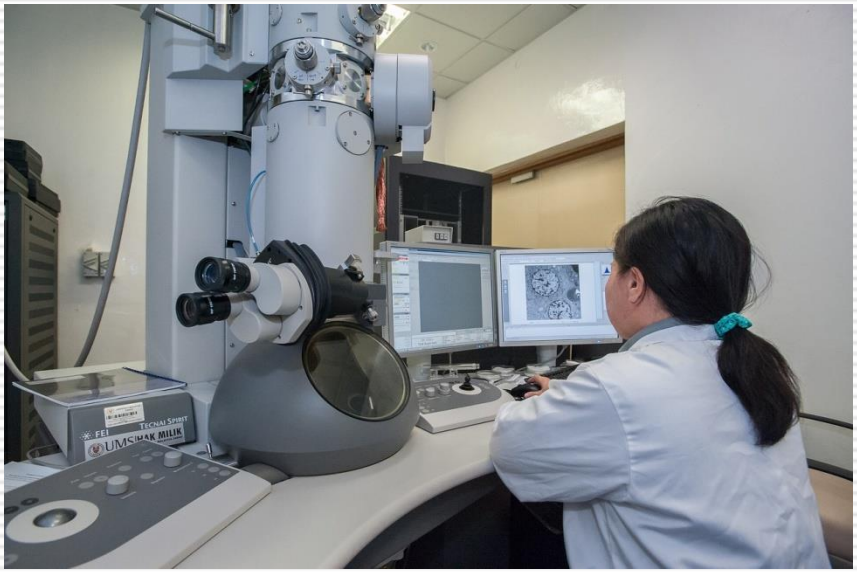

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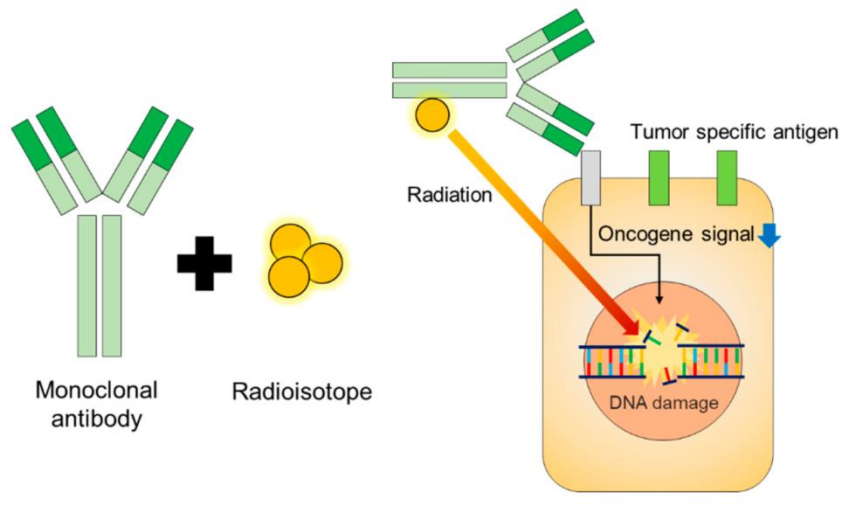
Biomedical:
ion beam cancer therapy,
targeted radionuclide therapy



J. Zaheer, H. Kim, Y.-J. Lee, J. S. Kim, S. M. Lim, M. Sang, *Int. J. Molec. Sciences* **20** (2019) 5579

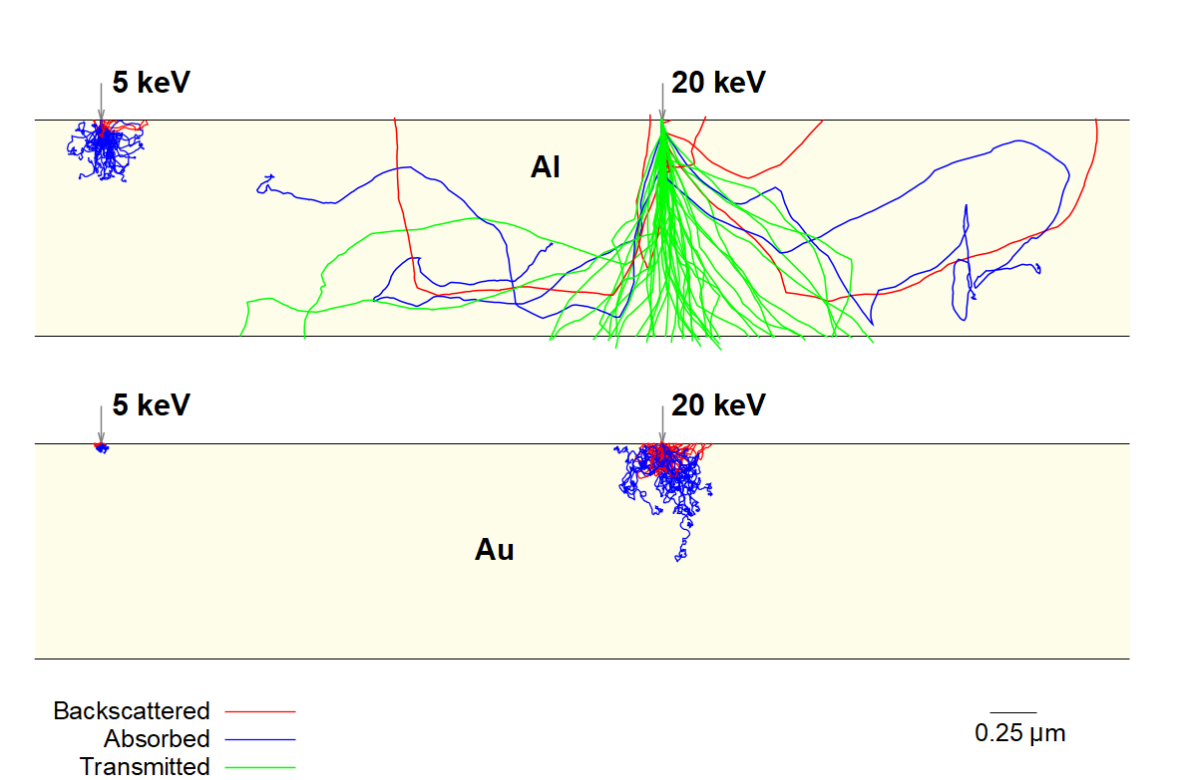
Monte Carlo simulations to increase knowledge and optimise applications

- Electrons behaviour for ↓↓E.
  - Deposition of dose.

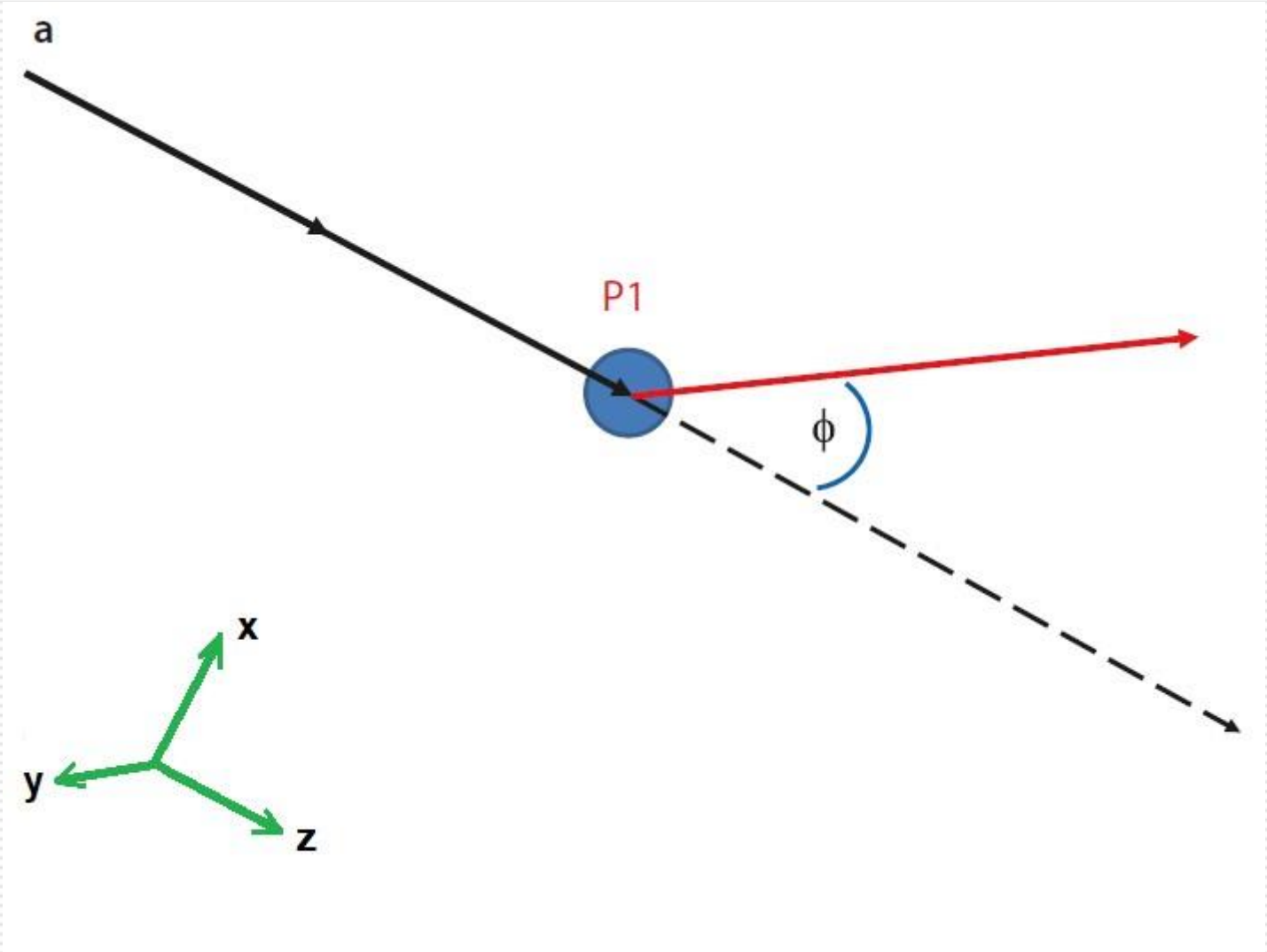
$$\eta_B = \frac{\#\ of\ backscattered\ e^-}{\#\ of\ total\ e^-}$$

$$\eta_T = \frac{\#\ of\ transmitted\ e^-}{\#\ of\ total\ e^-}$$

$$\eta_A = \frac{\#\ of\ absorbed\ e^-}{\#\ of\ total\ e^-}$$



Our Monte Carlo code



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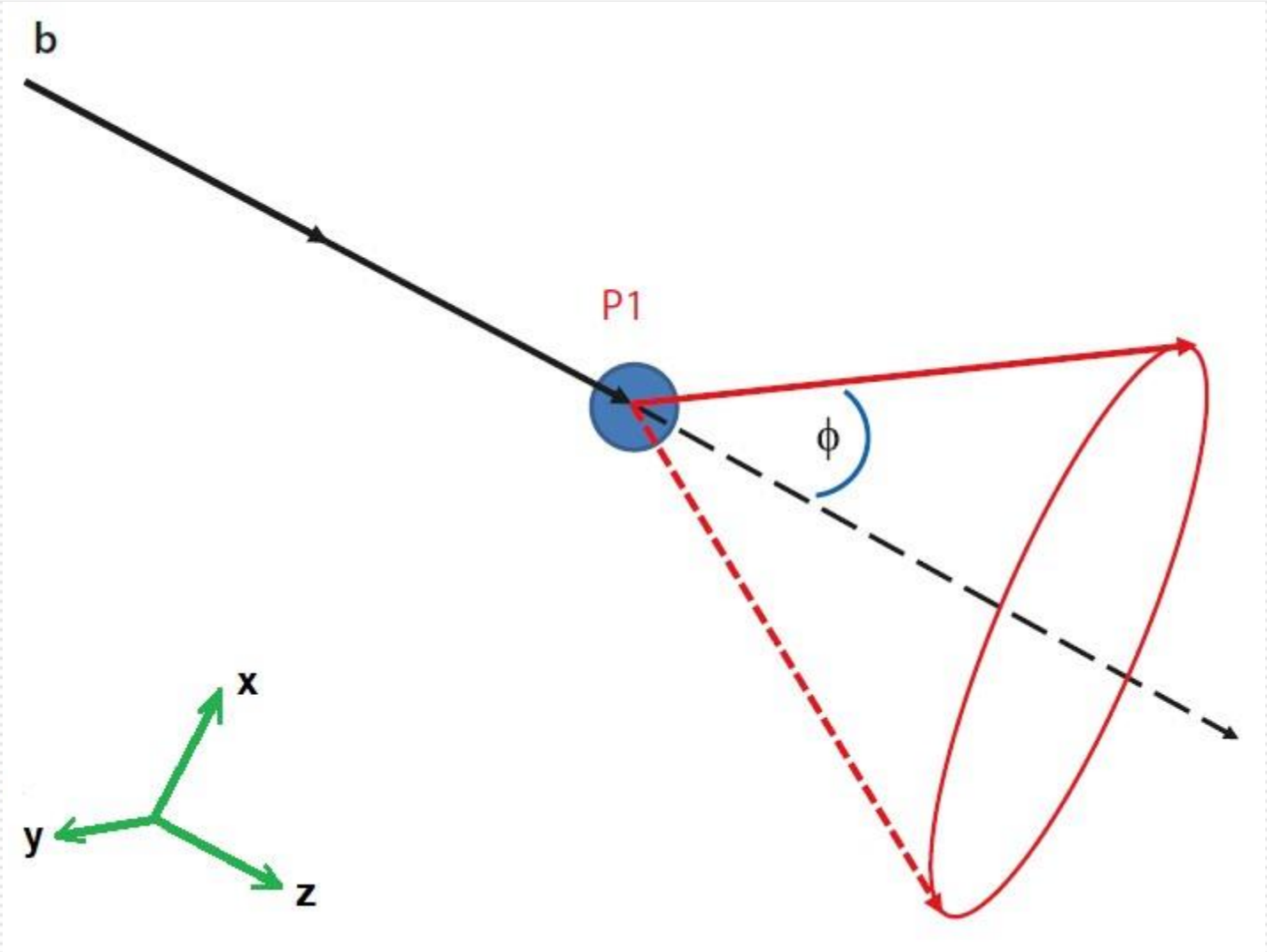

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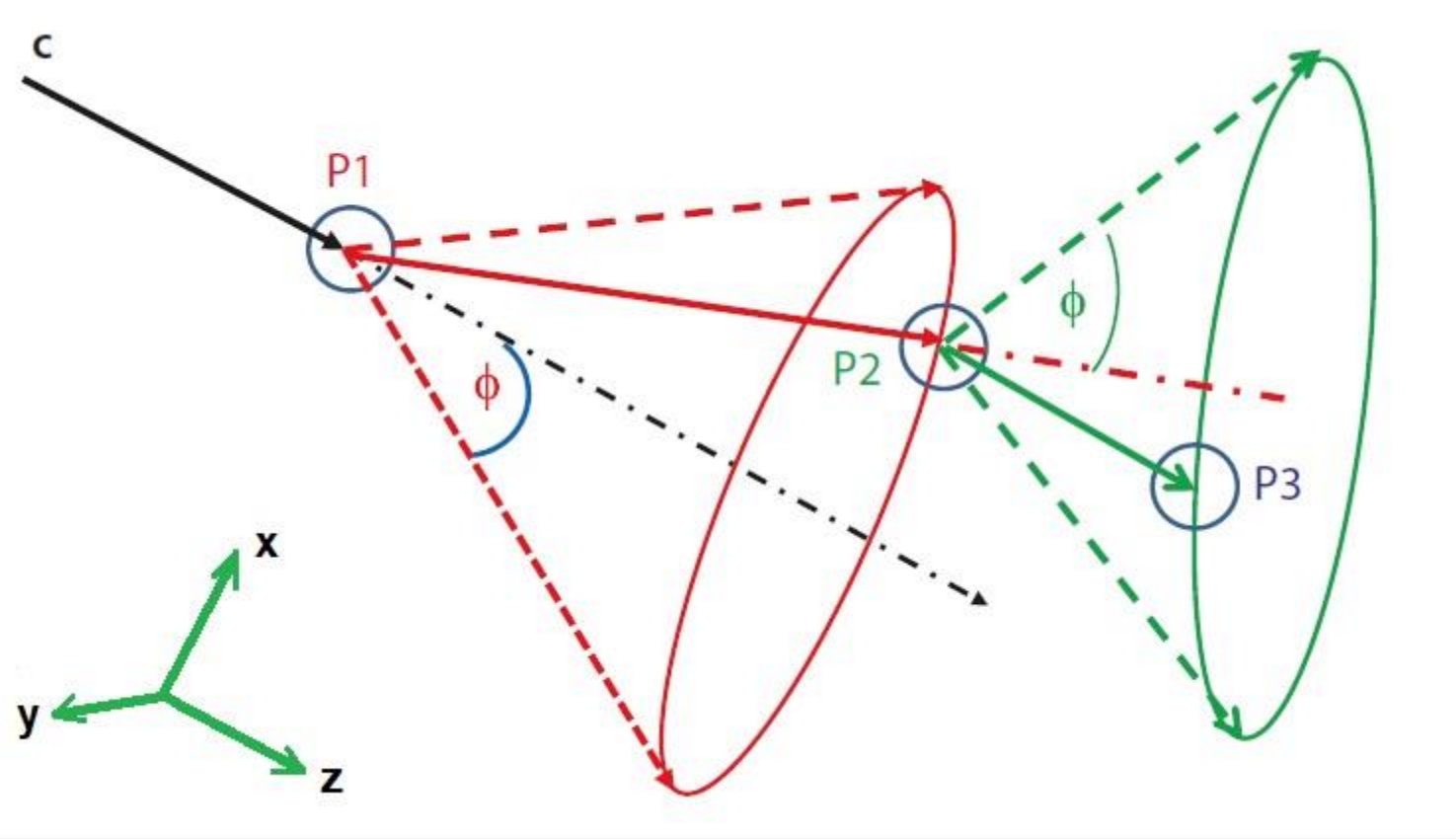

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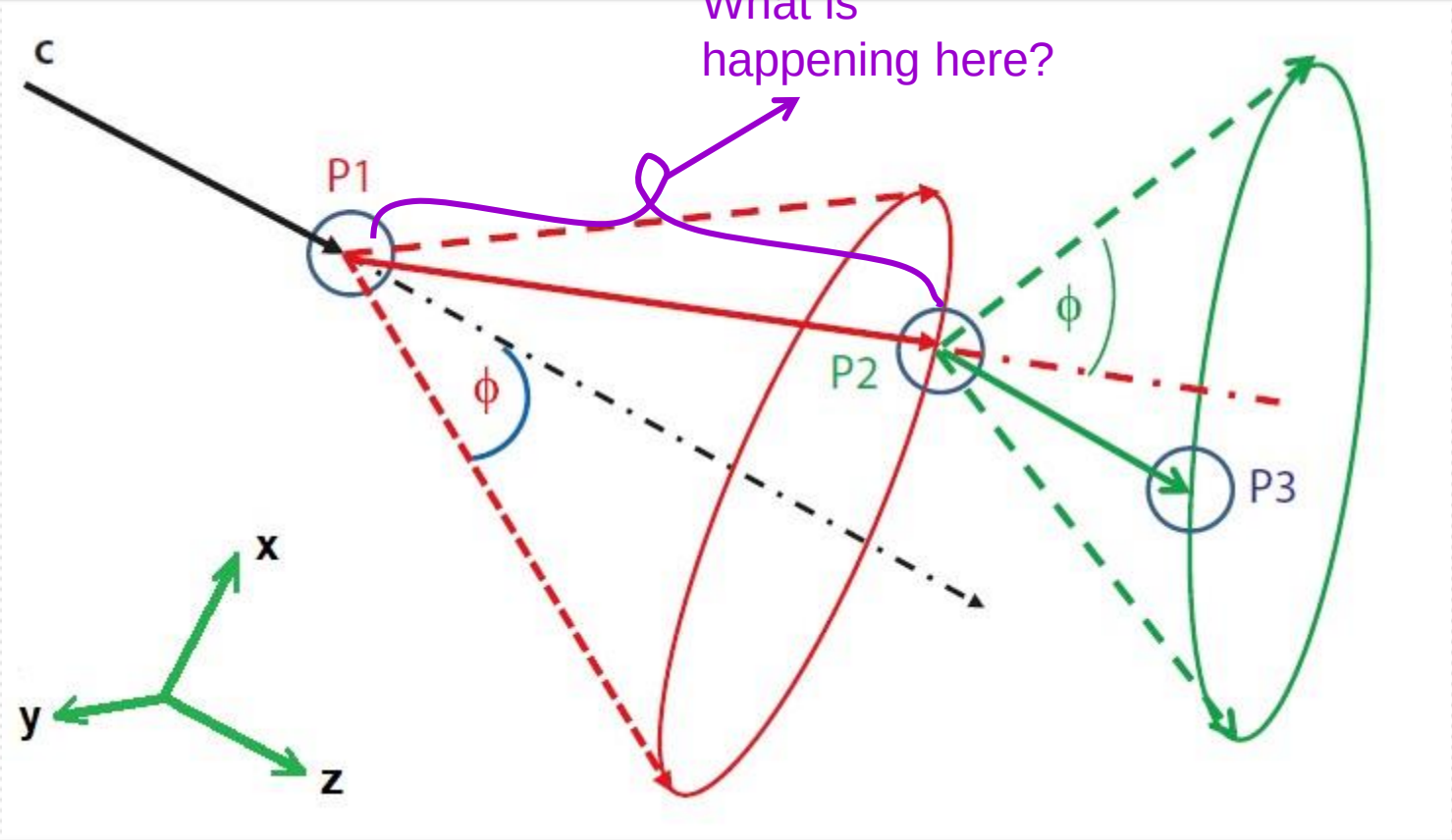
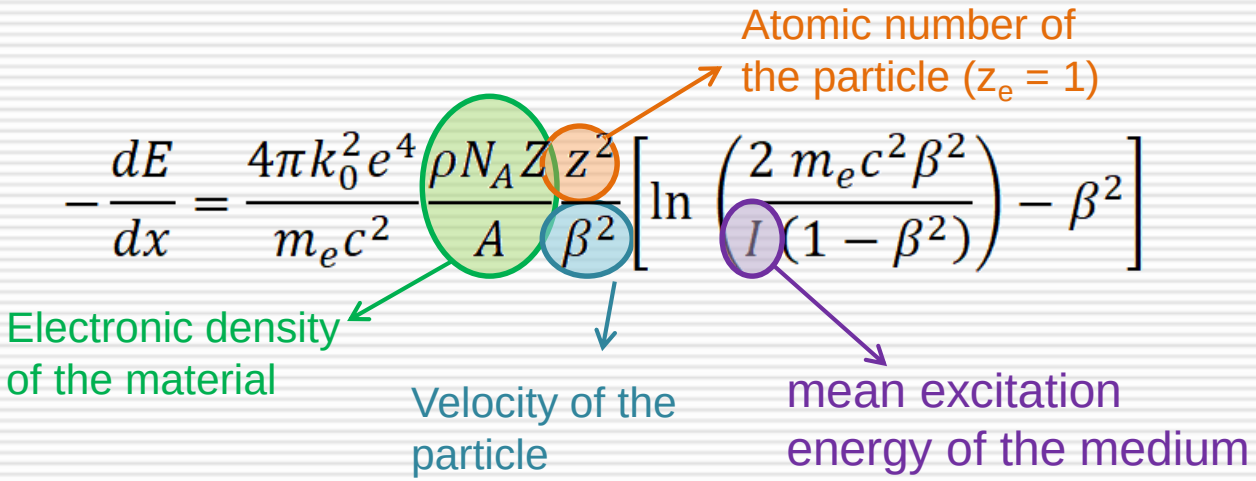


Stopping power formalism

- 1930s: Quantum Mechanics.
- Bethe formula (SI units):

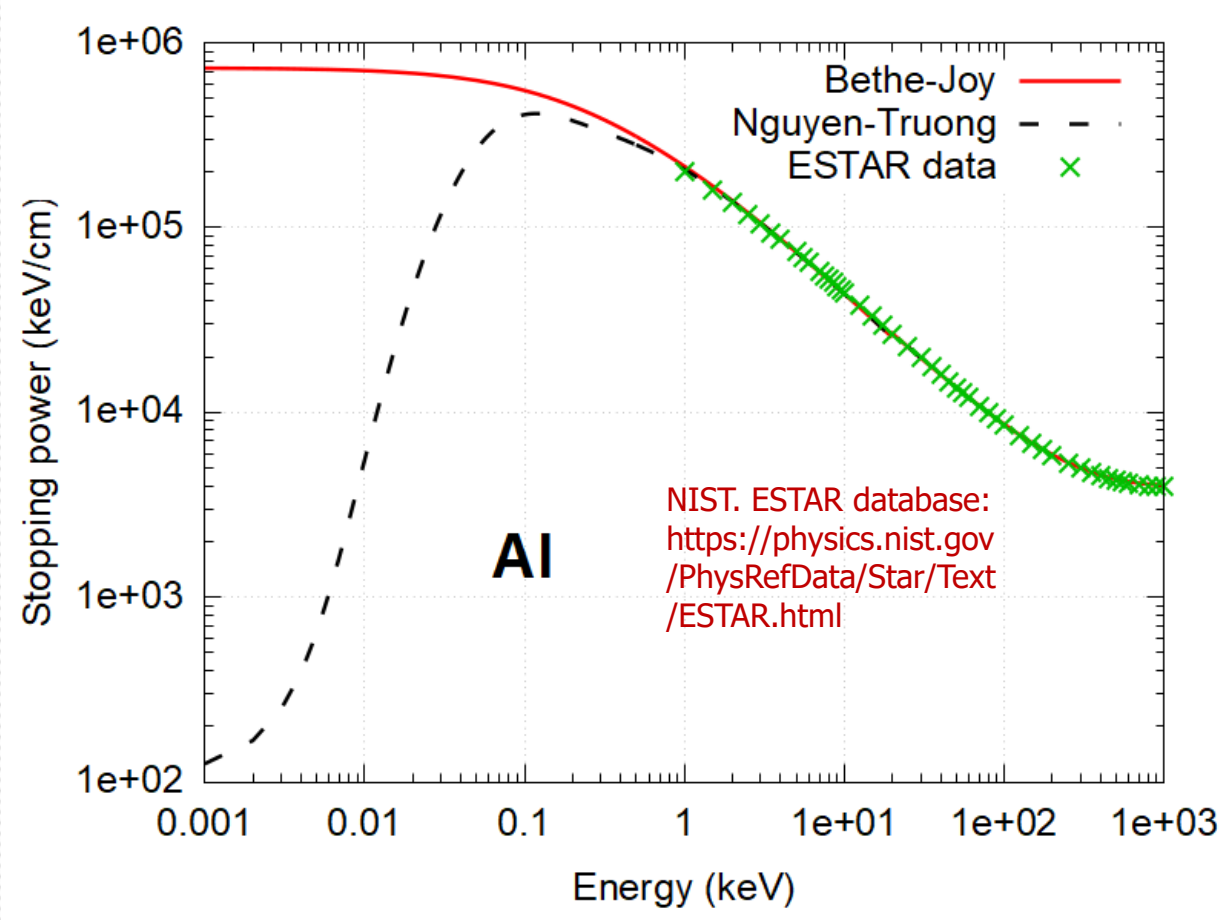


Turner, J. *Atoms, Radiation and Radiation Protection* (Wiley-VCH, 2007).

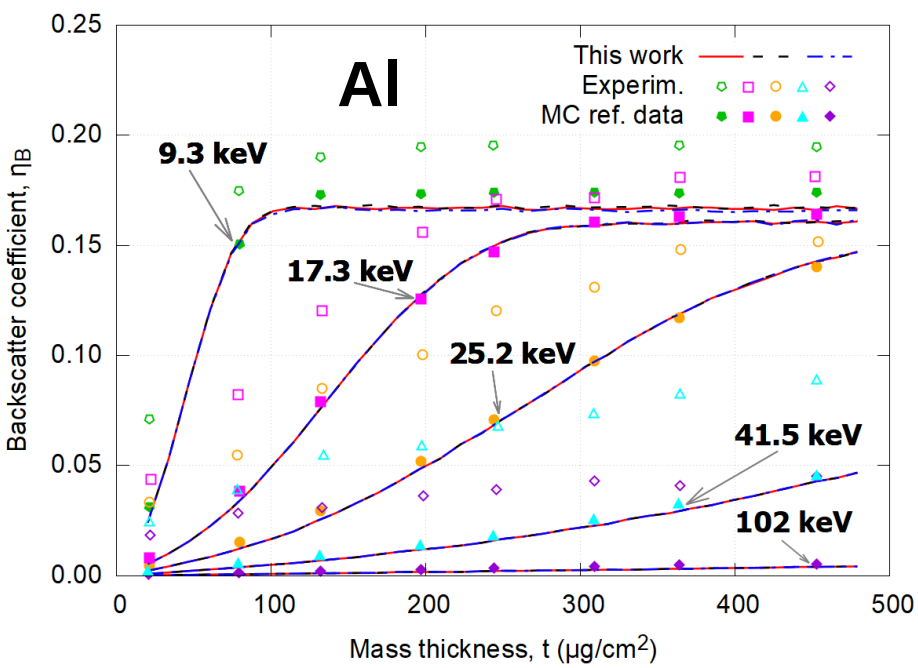
- Empirical modifications: Bethe-Joy, Nguyen-Truong.
- Other: dielectric formalism. ← **More accurate**

Stopping power results

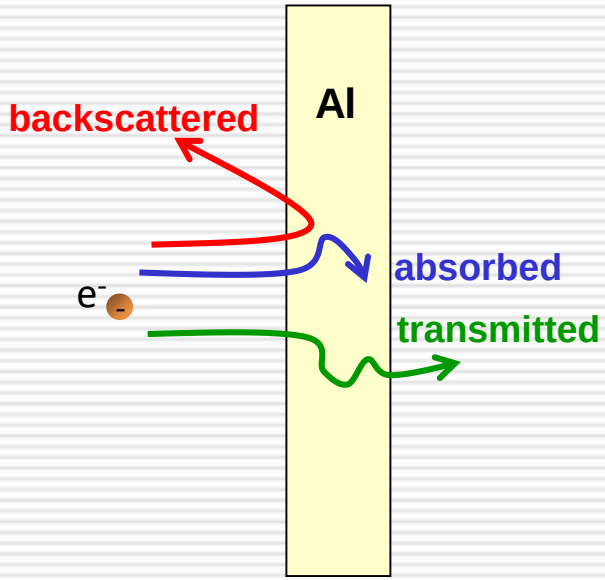
- Great agreement for ↑E.
- Differences between models for ↓↓E.



Dependence on mass thickness of backscatter and transmission coefficients



- More differences for:
  - ↓↓E.
  - Experimental data.



M. Attarian Shandiz, F. Salvat, R. Gauvin, *Scanning.* **38** (2016) 475-491

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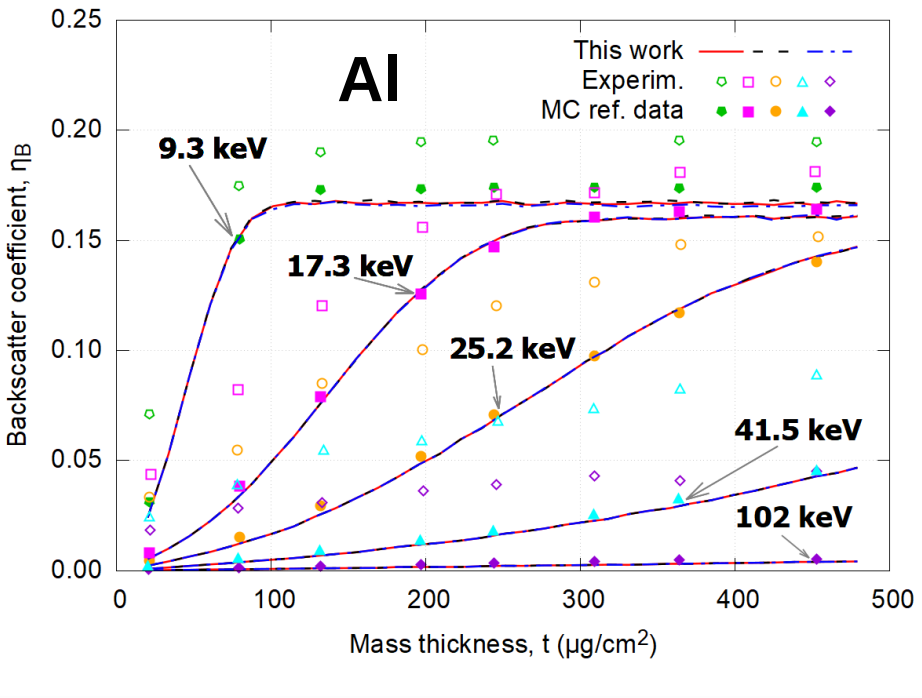

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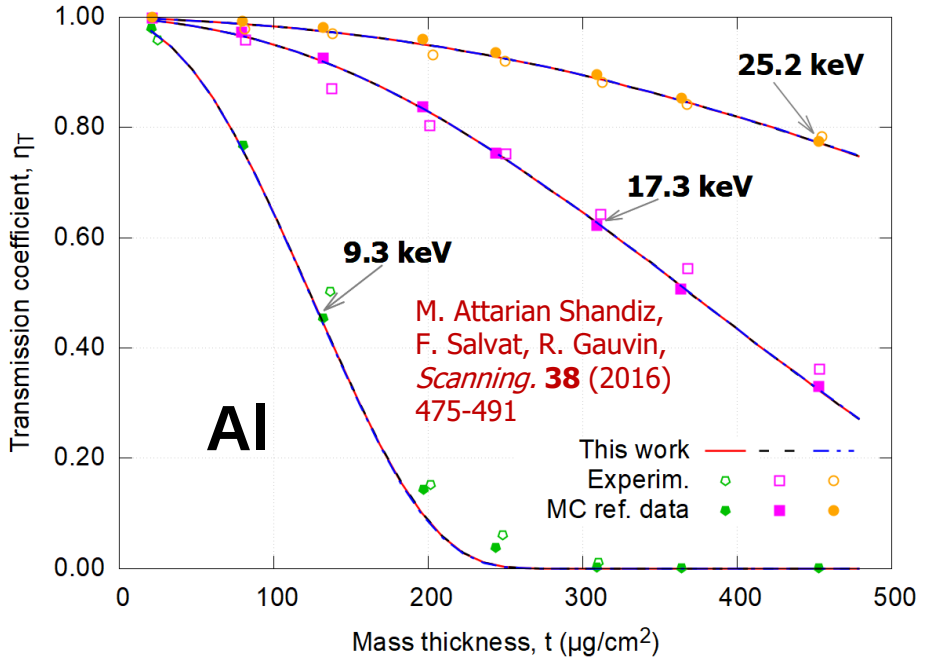
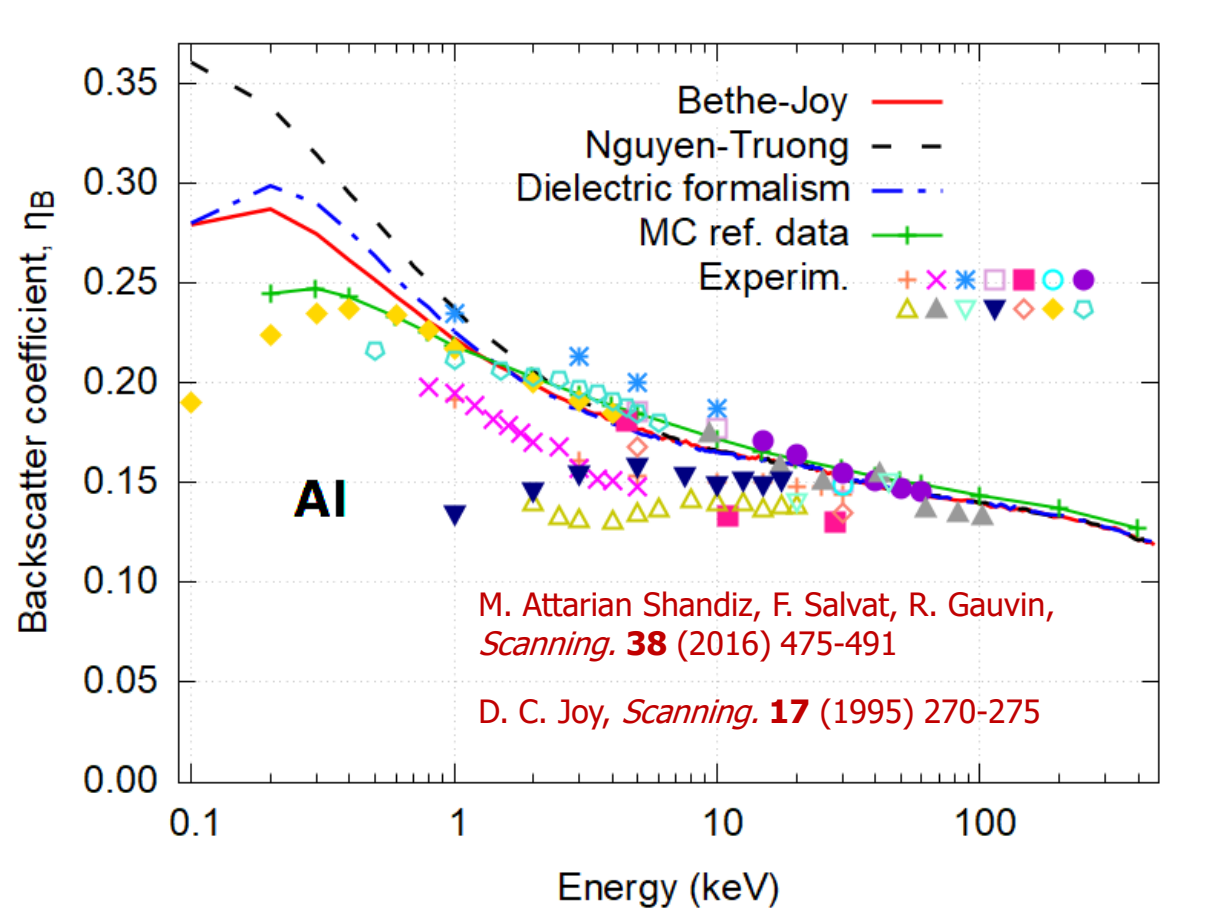
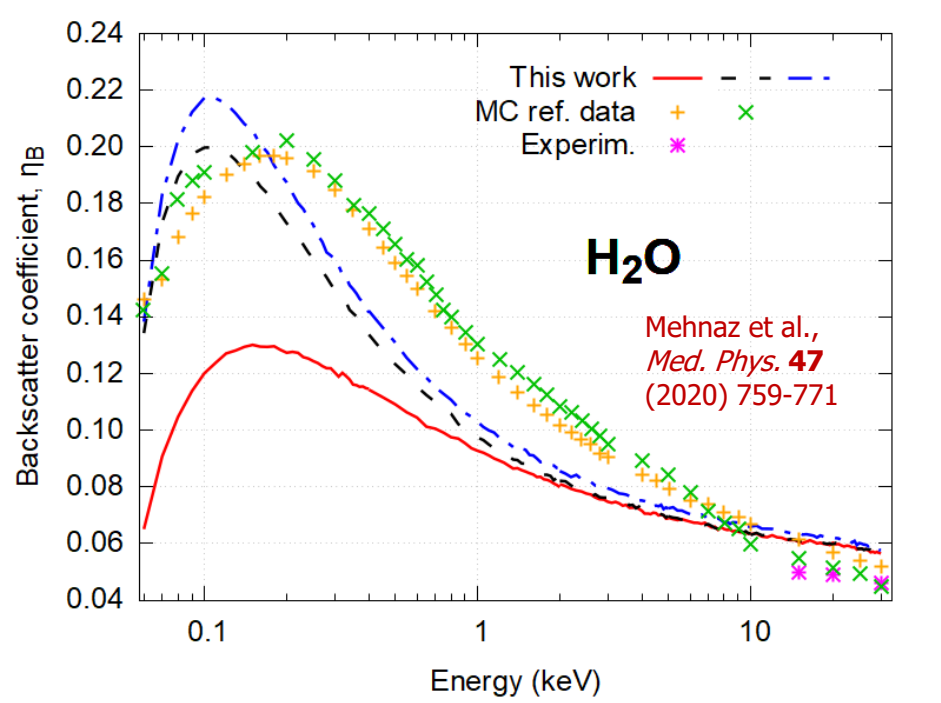


Backscatter coefficient vs. E for elements

- For infinite foils.
- Differences among models for ↓↓E.



Backscatter coefficient vs. E for organic materials



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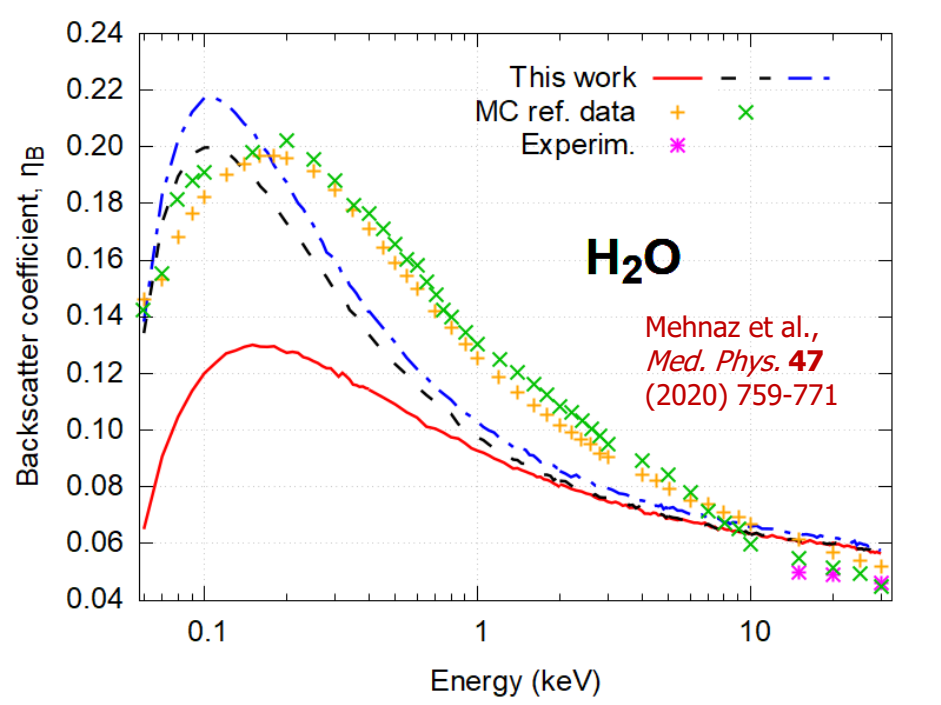

- Disagreement for water.

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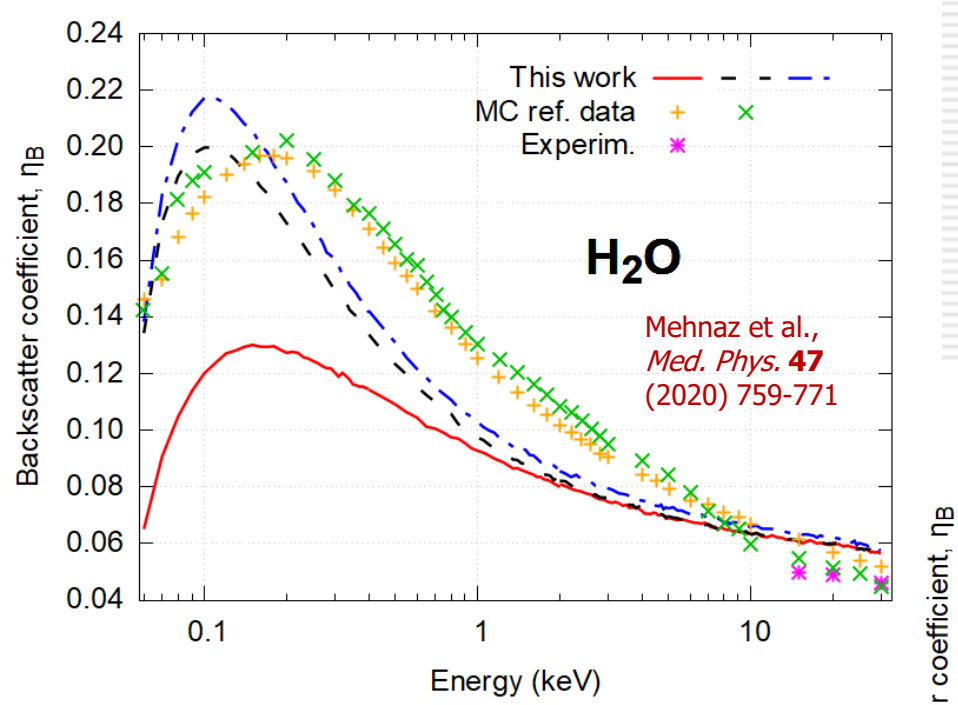

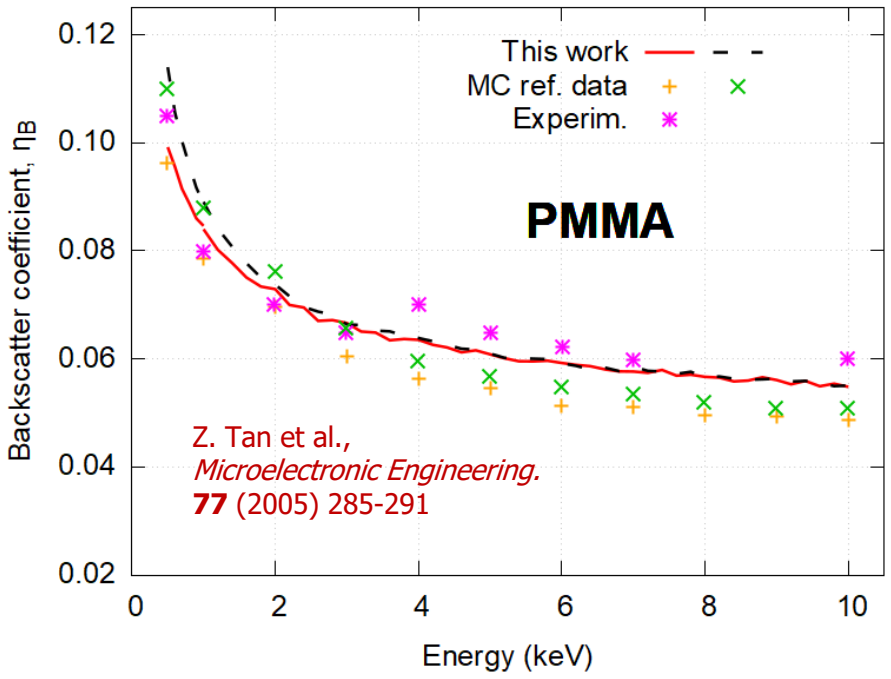

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Ana María Zamora-Vinaroz anamaria.zamorav@um.es

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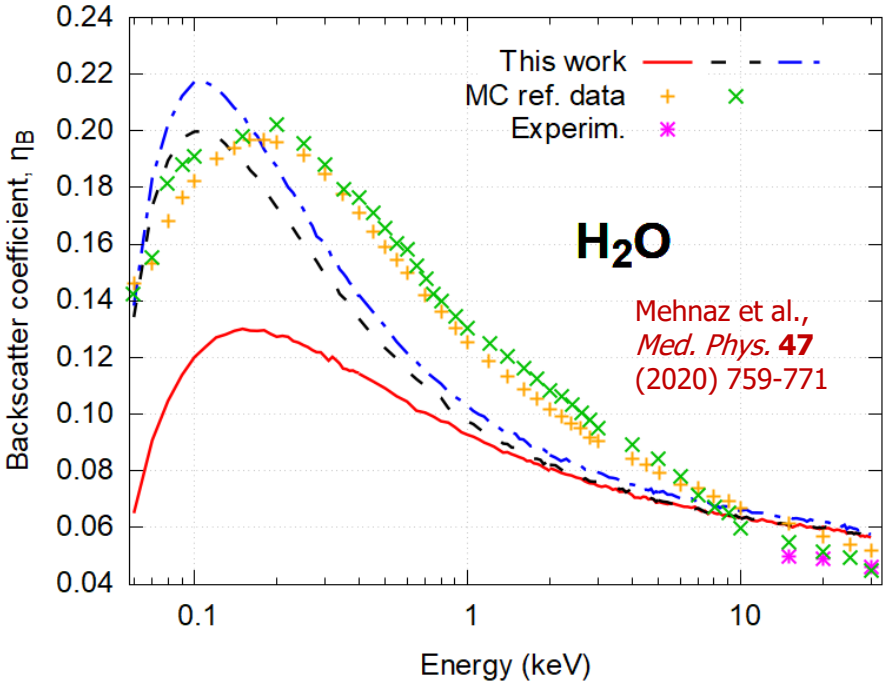

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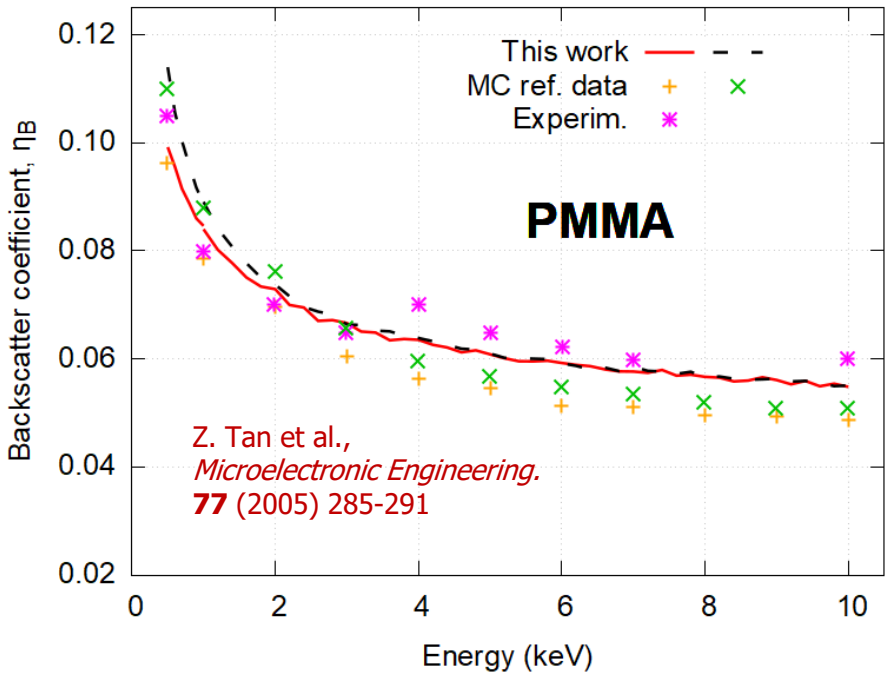
- Agreement for PMMA.



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Conclusions

- Several applications of electron-matter interaction:
  - Electron microscopy, material surface analysis…
  - Radiotherapy.
- Monte Carlo simulation: useful tool:
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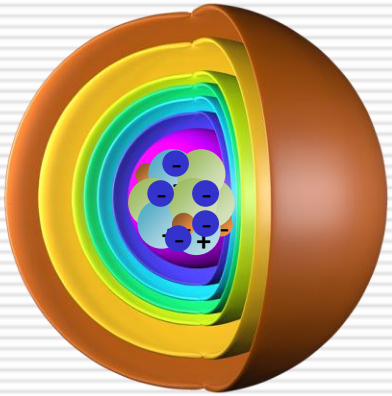

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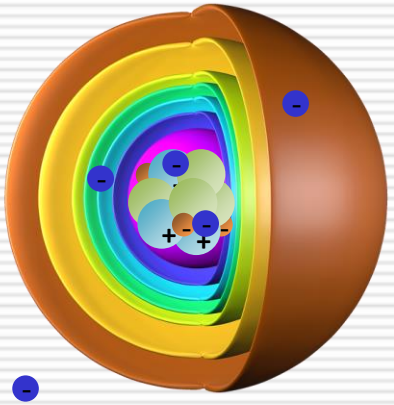

Thank you very much for your attention!

Ministerio de Ciencia, Innovación y Universidades:
Project PID2021-122866NB-I00 (2022-2025)
"Nanoscale Biodamage induced by Swift Ions: towards a detailed Modelling and Simulation"

Región de Murcia

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Región de Murcia

Fundación Séneca (Región de Murcia):
Project 22081/PI/22 (2023-2025)
"Energetic Particles Against Cancer: Detailed Simulations For A Better Use"

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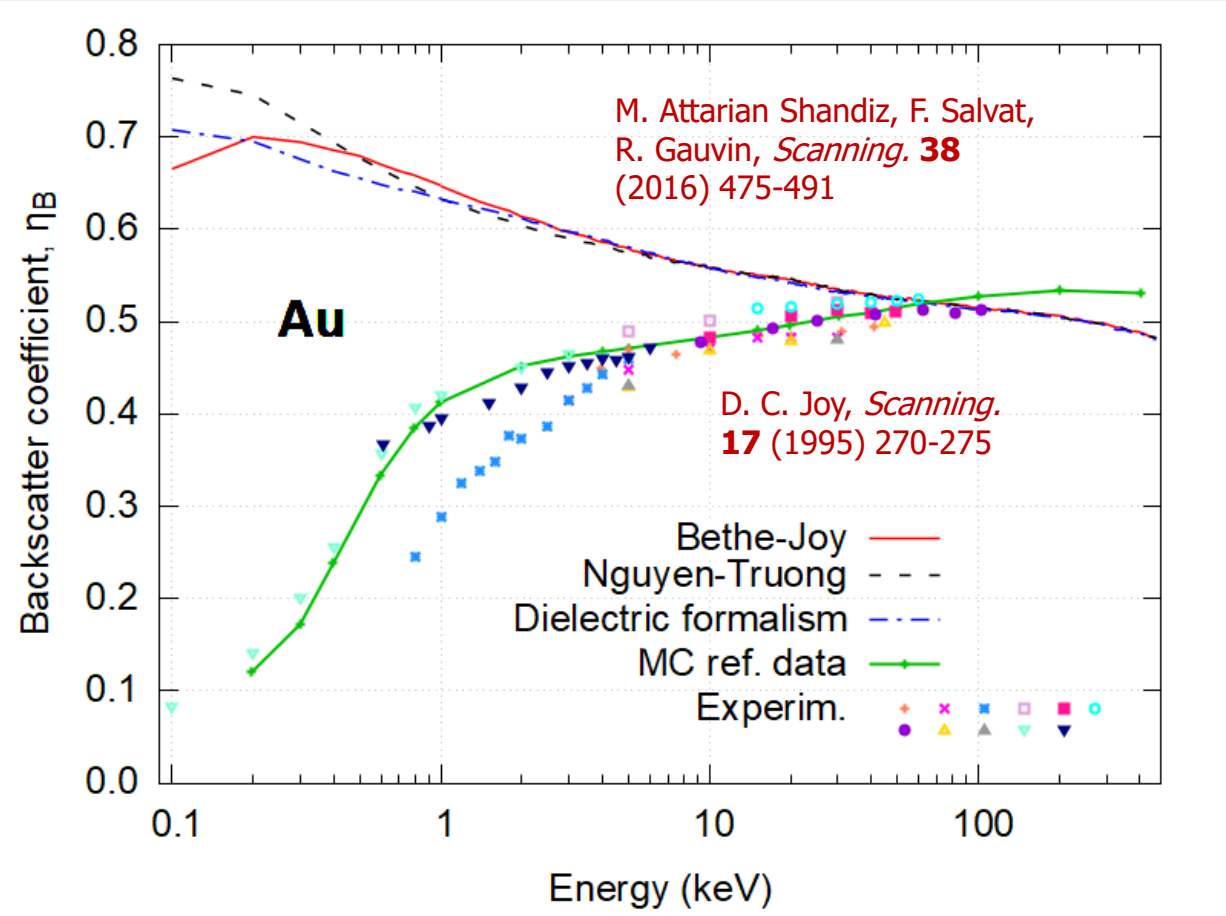

Bad for gold, why?

Backscatter coefficient vs. Z for different E

- Explanation of bad behaviour for ↑Z and ↓↓E.
- Another model for elastic cross sections for ↑Z.