

# From Hadrons to Therapy: Fundamental Physics Driving New Medical Advances

Contribution ID: 35

Type: **not specified**

## A simple procedure to generate cross section data for Monte Carlo simulations from Quantum Chemistry calculations. Example applications to Methacrylic acid.

*Monday 5 September 2022 16:55 (40 minutes)*

Monte Carlo Simulations of electrons in condensed matter require the knowledge of cross section data [1]. We present a simple procedure, which allows to generate a consistent set of cross sections for Monte Carlo simulations from parameters, which can be obtained from Quantum Chemistry calculations with standard software as for example the program package Gaussian.

We show how the cross sections can be converted into probabilities. We demonstrate their usage in Monte Carlo simulations of the secondary electron yield from Methacrylic acid (MAA). MAA is the main component of the gel called MAGIC (methacrylic and ascorbic acid in gelatin initiated by copper), which is a gel for radiation dosimetry [3]. In the gas-phase MAA has four different conformers. Each of them gives a different secondary electron yield.

### REFERENCES

- [1] M. Dapor, Transport of Energetic Electrons in Solids, 3rd ed. (Springer Nature, 2020).
- [2] Gaussian 16, Revision C.01, M. Frisch et al., Gaussian, Inc., Wallingford CT, (2016)
- [3] J. J. Luci, H. M. Whitney, J. C. Gore, Phys Med Biol.52, N241(2007)

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**Session Classification:** New developments in the modelling of radiation propagation and effects

**Track Classification:** Modelling of radiation propagation, effects and radiobiology