TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

Measurement and modelling of thermal neutron cross sections for neutron transport simulations

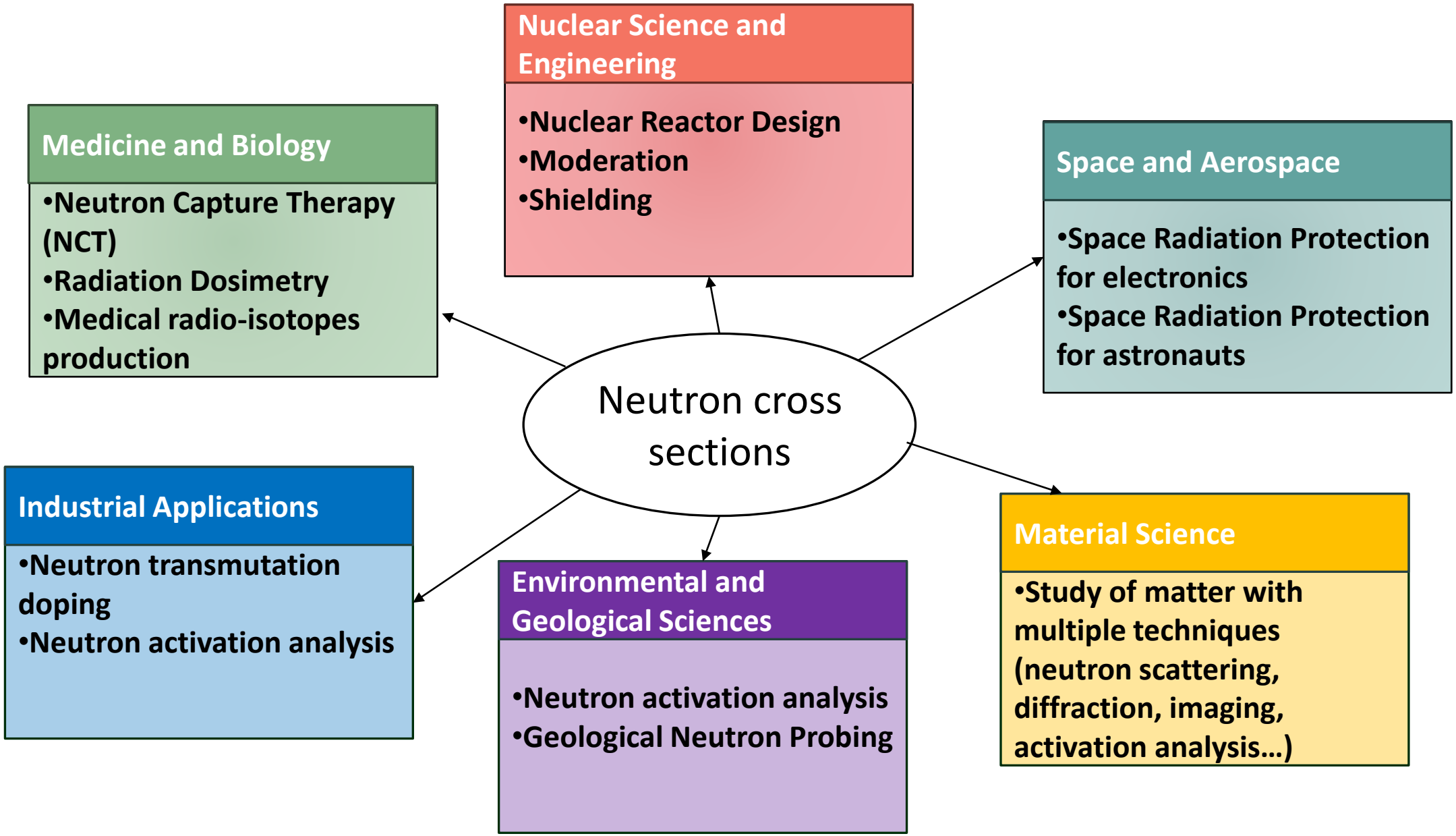
PhD student

Margherita Simoni

Supervisors

Prof. Roberto Senesi

Prof. Giovanni Romanelli


Nuclear Science and Engineering
•Nuclear Reactor Design
•Moderation
•Shielding
Medicine and Biology
•Neutron Capture Therapy (NCT)
•Radiation Dosimetry
•Medical radio-isotopes production
Space and Aerospace
•Space Radiation Protection for electronics
•Space Radiation Protection for astronauts
Neutron cross sections
Industrial Applications
•Neutron transmutation doping
•Neutron activation analysis
Environmental and Geological Sciences
•Neutron activation analysis
•Geological Neutron Probing
Material Science
•Study of matter with multiple techniques (neutron scattering, diffraction, imaging, activation analysis…)

Monte Carlo transport simulations

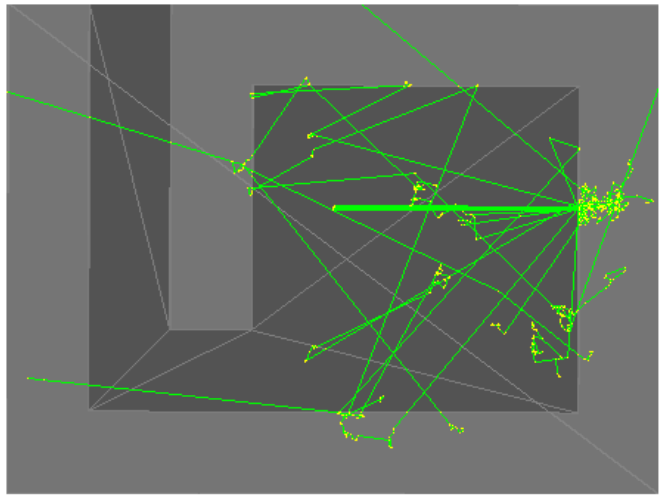
Thermal neutron Cross Sections (TCSs) are a fundamental ingredient for the simulation and design of technical equipment

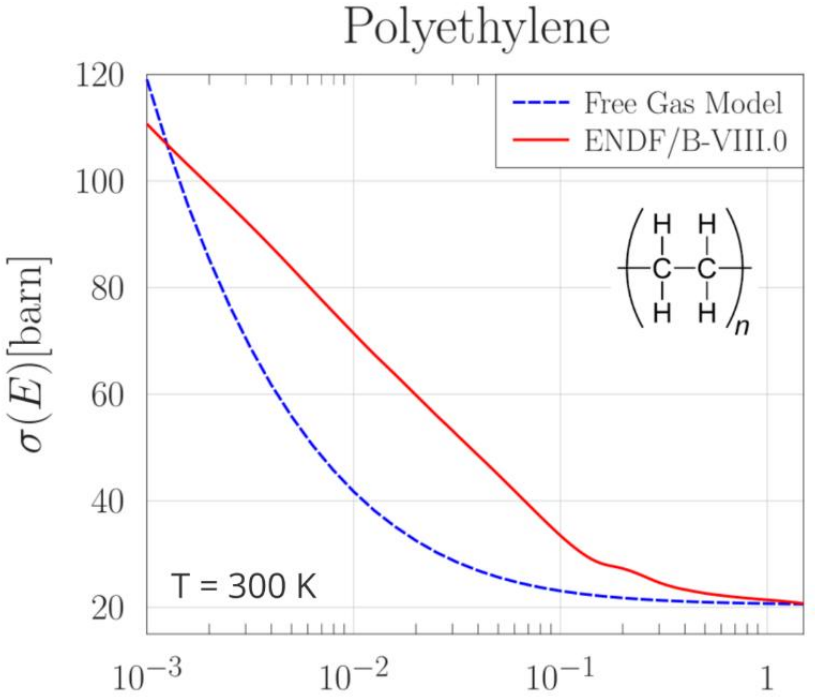
Safety measures have to be tailored to each specific case, to establish both **design** and **operating mode** of the device

FLUKA

GEANT4
A SIMULATION TOOLKIT

MCNP
MONTE CARLO N-PARTICLE





Different molecules require different simulations, which can **become computationally expensive**, especially for **large molecules** and **disordered polymers**.

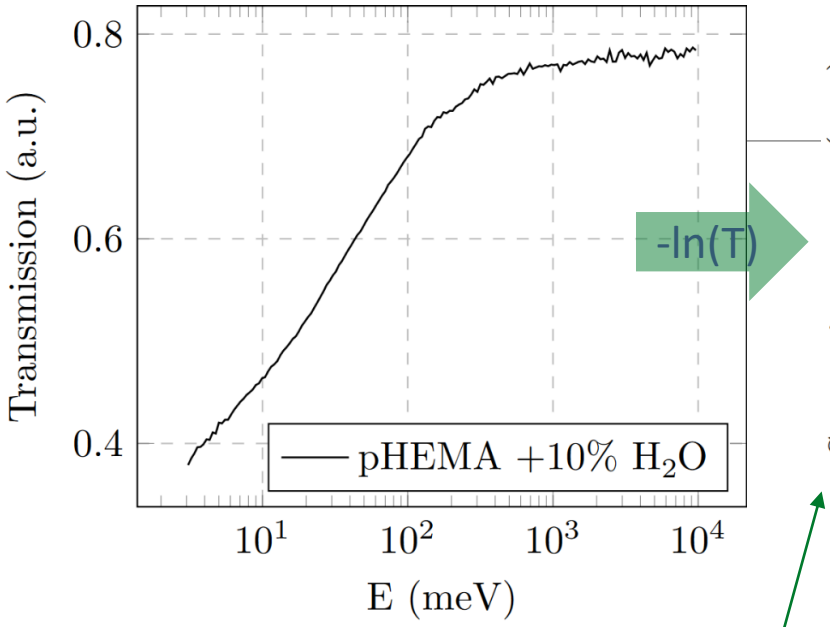
Thermal neutron cross sections models

1. Thermal neutron cross section of air: molecular rotations and magnetic scattering
2. Cross section of hydrated hydrogen-based materials
3. Cross section modelling for neutron imaging
4. Experimental validation of the scattering libraries for thermal neutron transport within moderators for BNCT
5. Use of CR-39 Dosimeters for the Imaging of Neutron Beam Profiles.

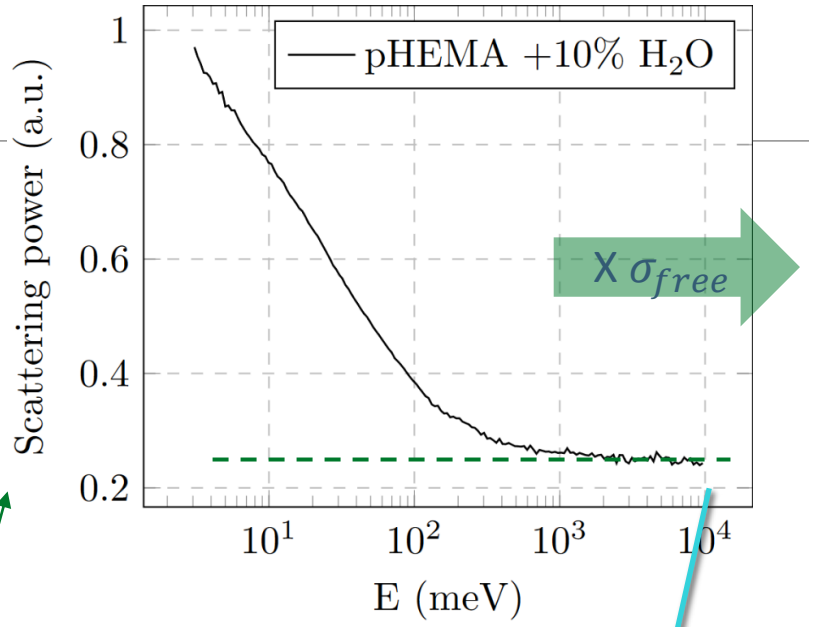
ISIS Neutron and Muon Source

UKRI Science and Technology Facilities Council

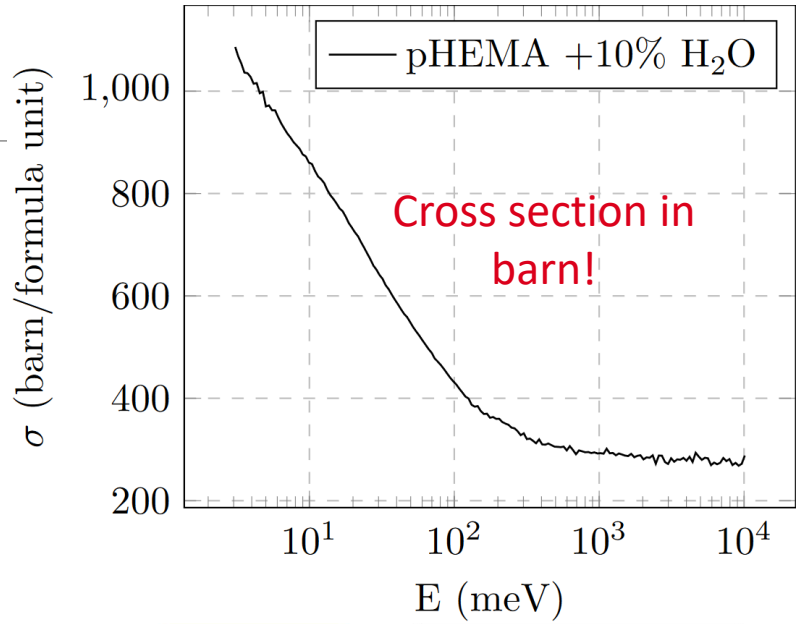
From neutron transmission to cross sections



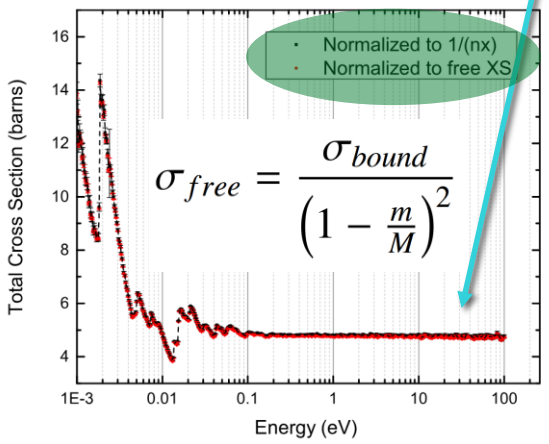
-ln(T)

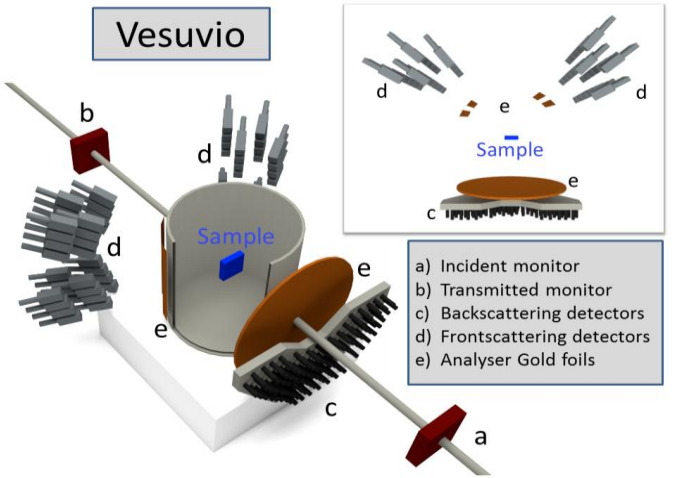


X σ_{free}



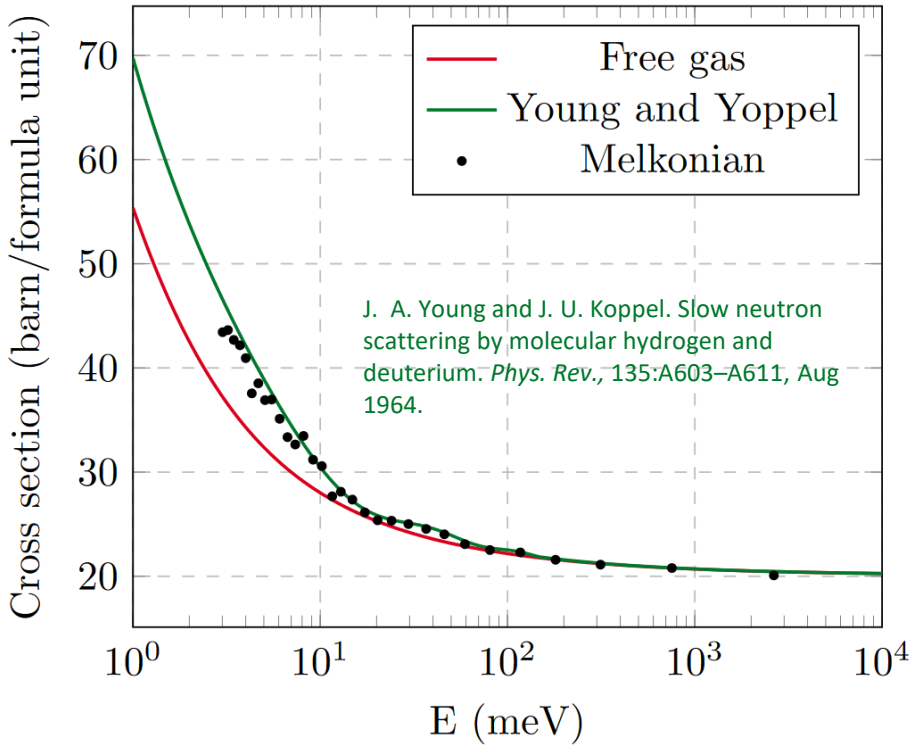
$$T(E,x) = \frac{I_t(E,x)}{I_0(E)} = e^{-Nx\sigma_T(E)}$$



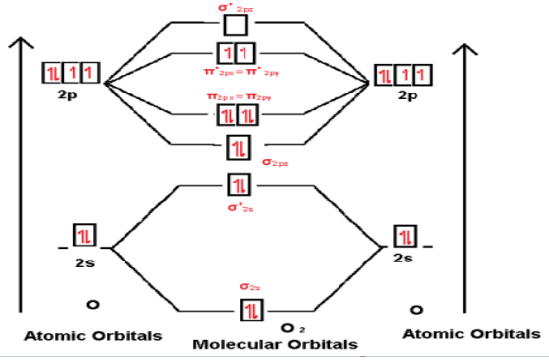


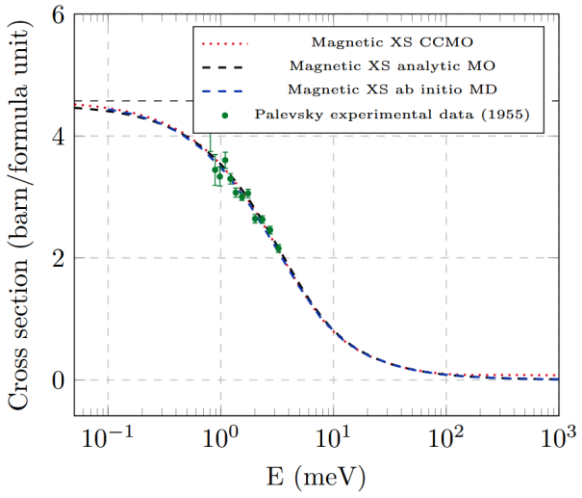
J.I. Robledo, J. et al. Measurement of neutron total cross sections at the VESUVIO spectrometer, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, https://doi.org/10.1016/j.nima.2020.164096.

Thermal neutron cross section of air: molecular rotations and magnetic scattering

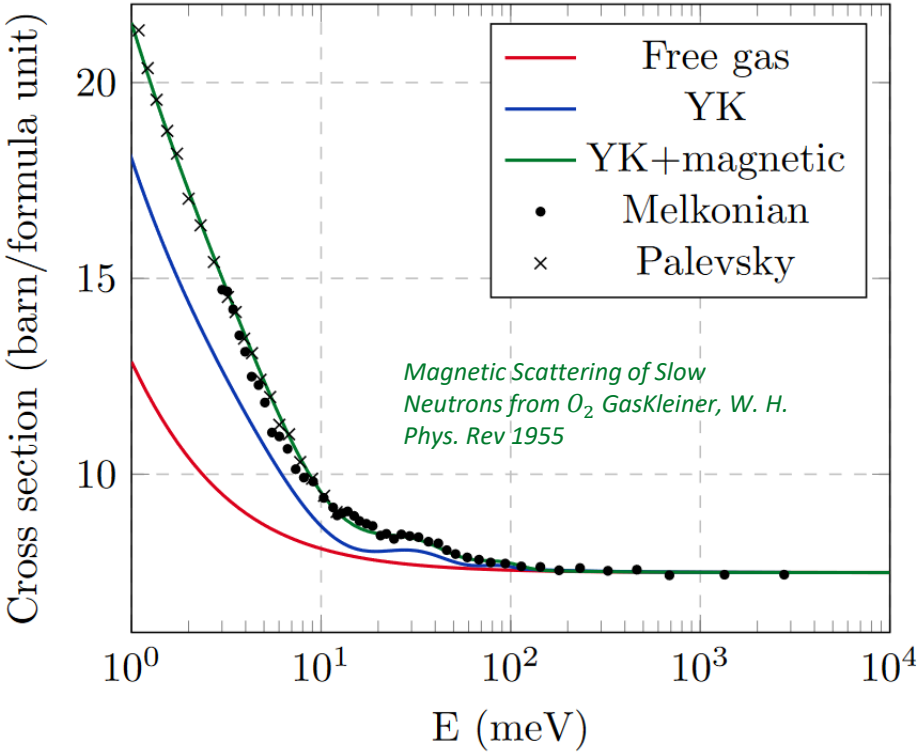


Neutron scattering cross section was estimated using **Young and Koppel model**, and compared to the free gas model and to experimental data from 1955.

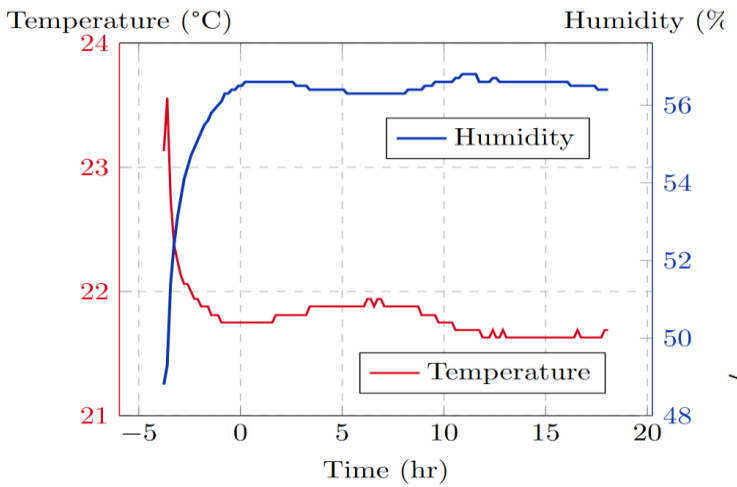


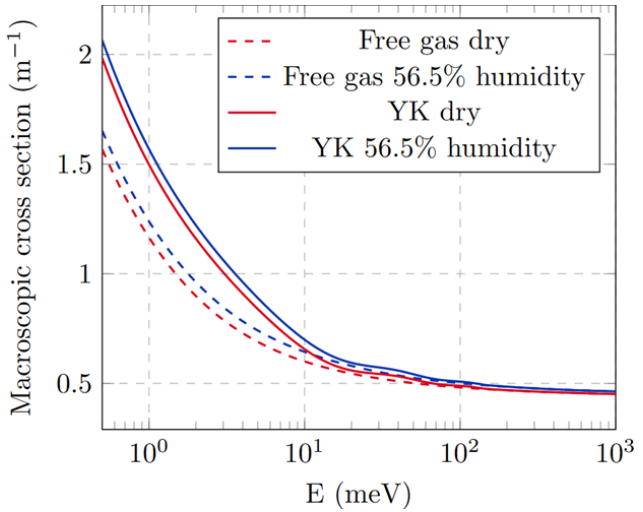


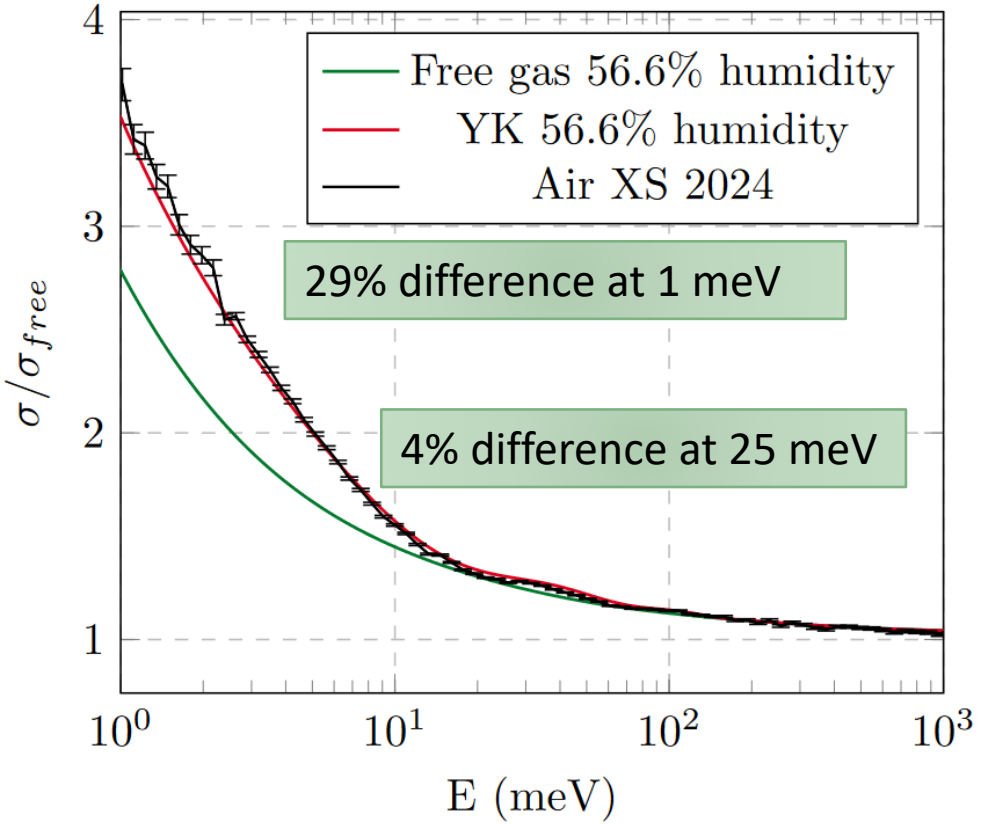
Young and Koppel model was not enough to reproduce O_2 cross section: Its paramagnetic behaviour need to be considered.



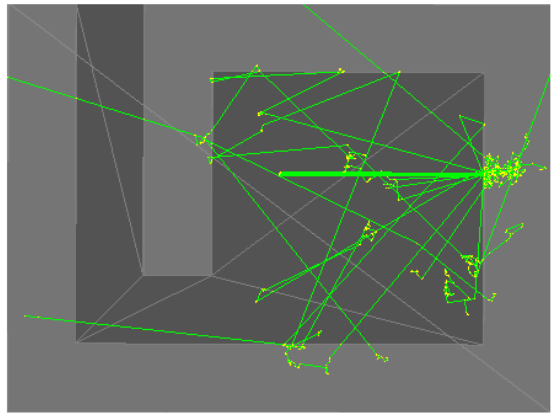
Thermal neutron cross section of air: molecular rotations and magnetic scattering





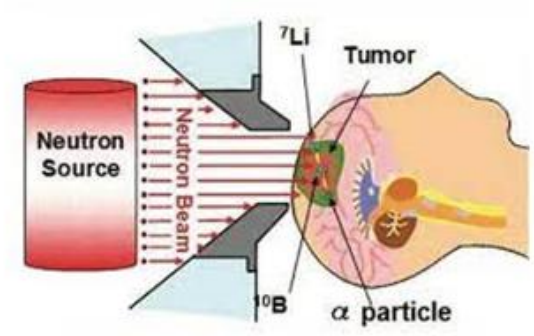


Next step: Integrating the model into Monte Carlo transport simulations to quantify its impact.



Experimental validation of the model was performed at the VESUVIO Spectrometer, ISIS neutron and muon source.

Cross section of hydrogen-based materials



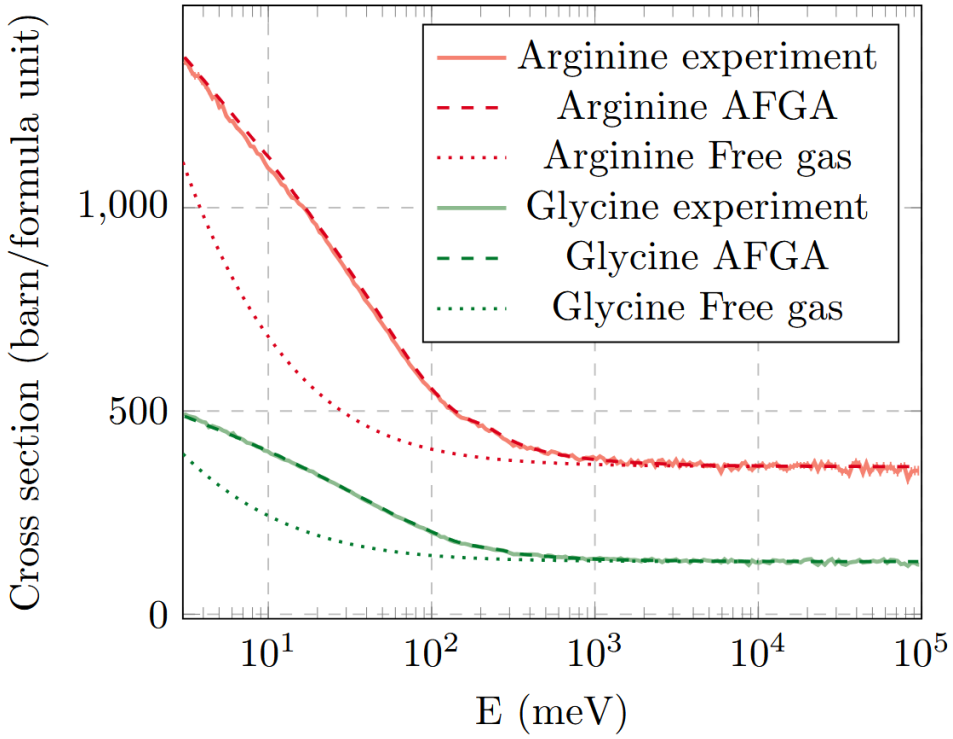
$^{10}B(n,\alpha)^{7}Li$

Reaction products destroy cancer cells

It is important to maximise the neutron dose that reaches the tumor and reduce the dose on healthy tissue. This requires to be able to simulate **neutron transport in the human body.**

AFGA: simplified **phenomenological approach** for the accurate calculation of thermal neutron cross sections of large organic molecules and polymers.

Uses a limited number of effective Vibrational Densities of States (VDoSs), representing the hydrogen dynamics of functional groups



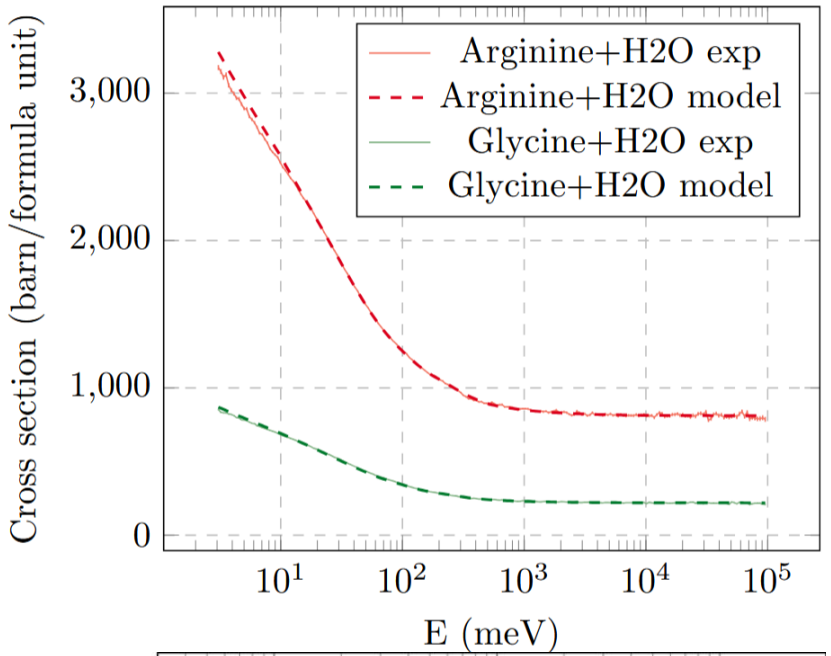
Romanelli g. et al. J Phys Condens Matter. 2021 May 31;33(28).PMID: 33906173.

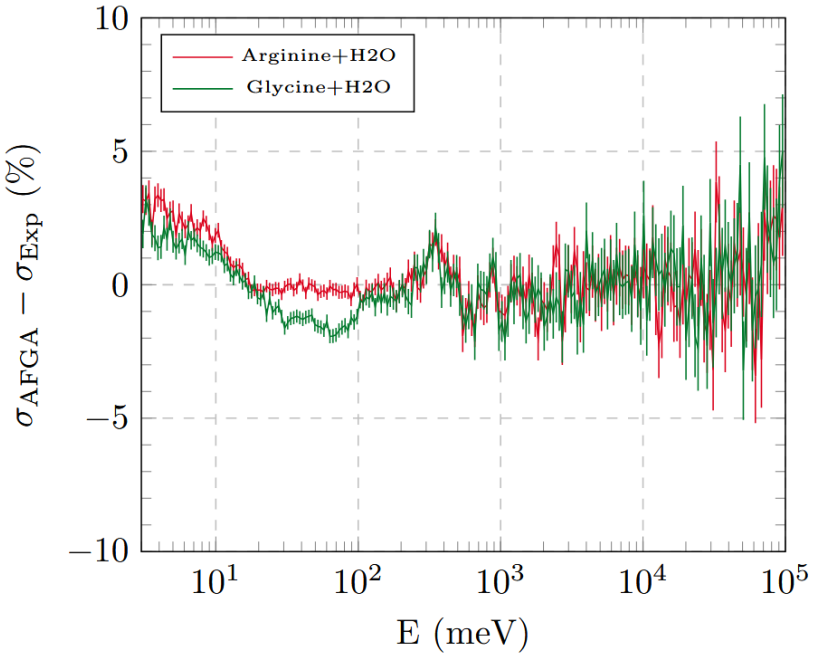
A model for hydrated amino acids and polymers

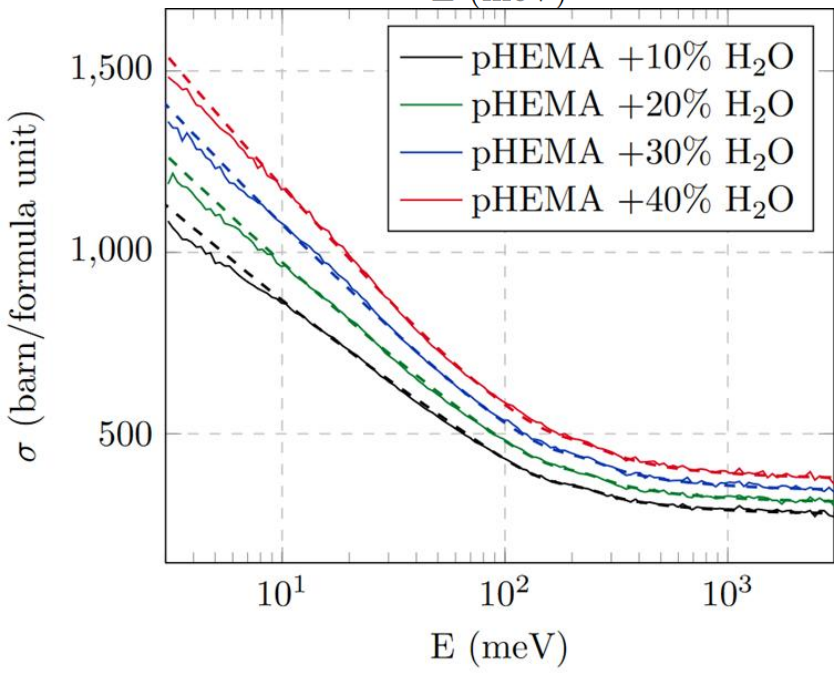
AFGA model

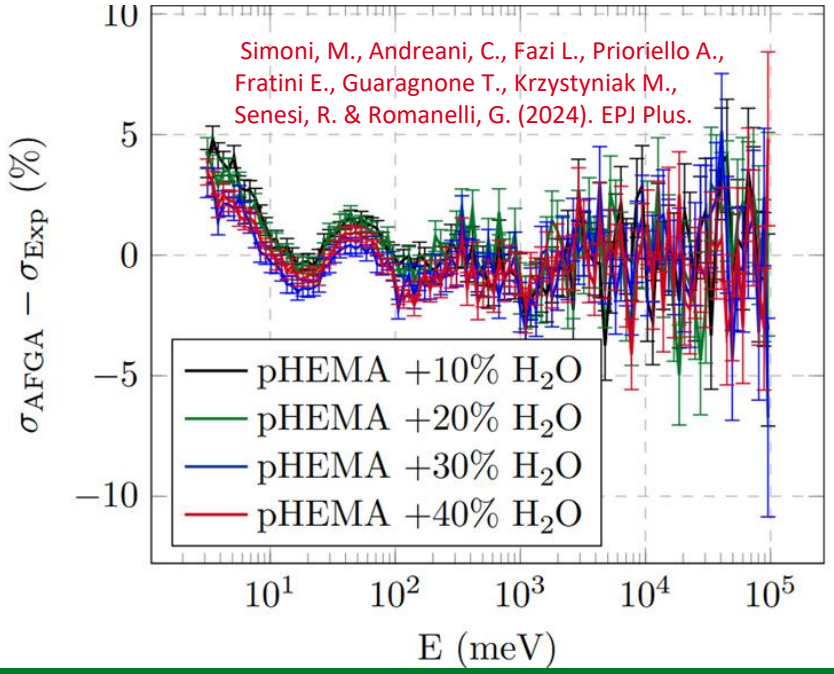
NC library for H2O

Differences between simulations and experimental data follow a specific trend, which contains informations on phenomena we did not take into account in the simulations, as **water confinement** and **water-polymer interactions**

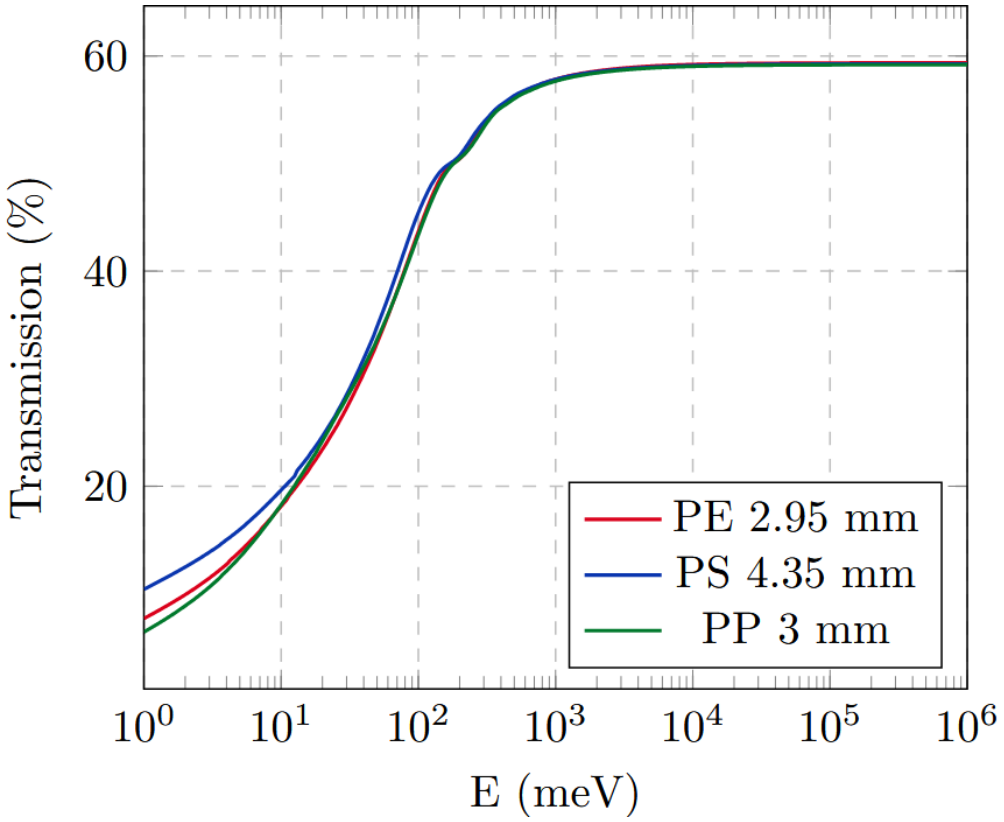






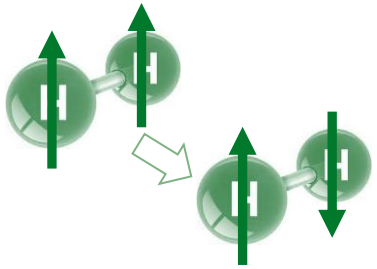


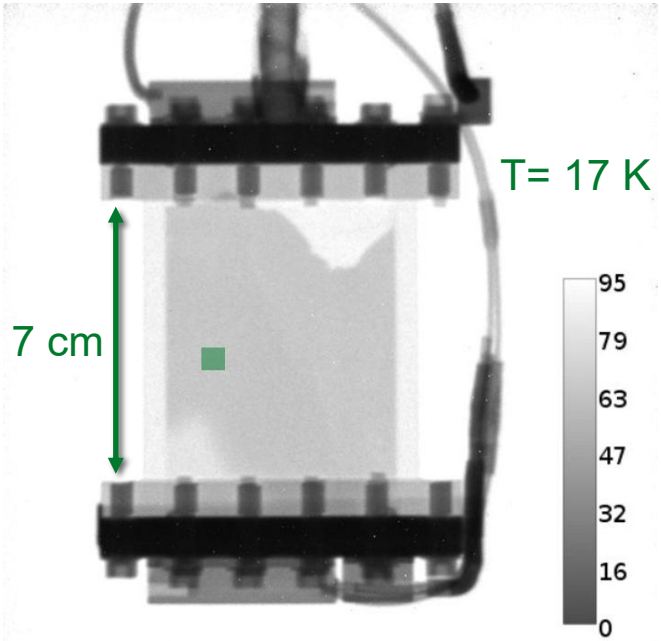
Cross section modelling for neutron imaging



AFGA for maximising the contrast in **energy selective neutron imaging** experiments on hydrogen-based materials

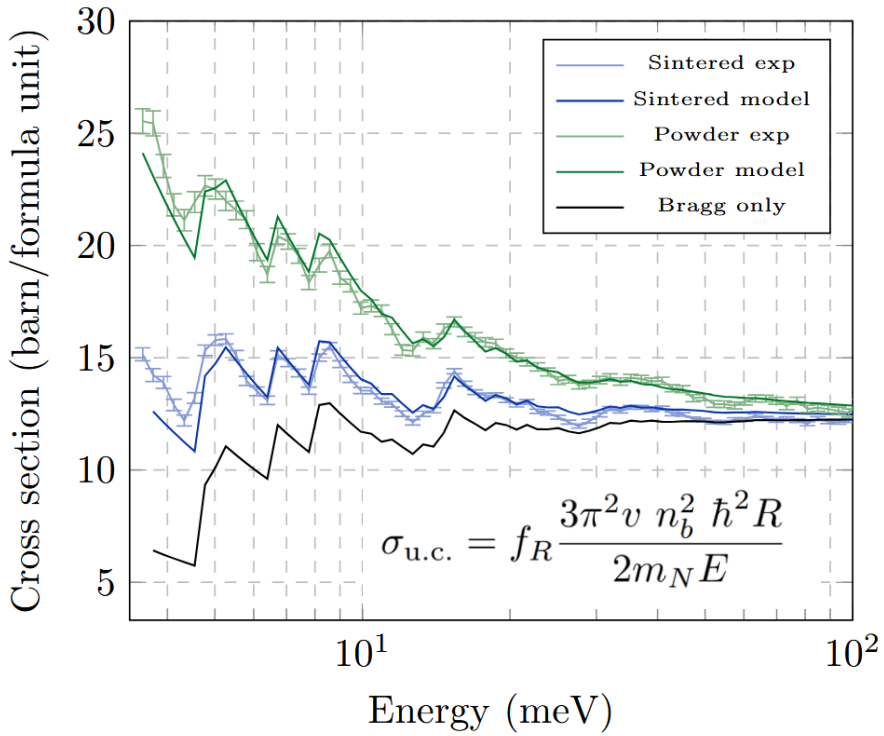
We exploited the significant difference in the neutron scattering cross sections of ortho and para hydrogen, to investigate the adsorption and conversion of H2.



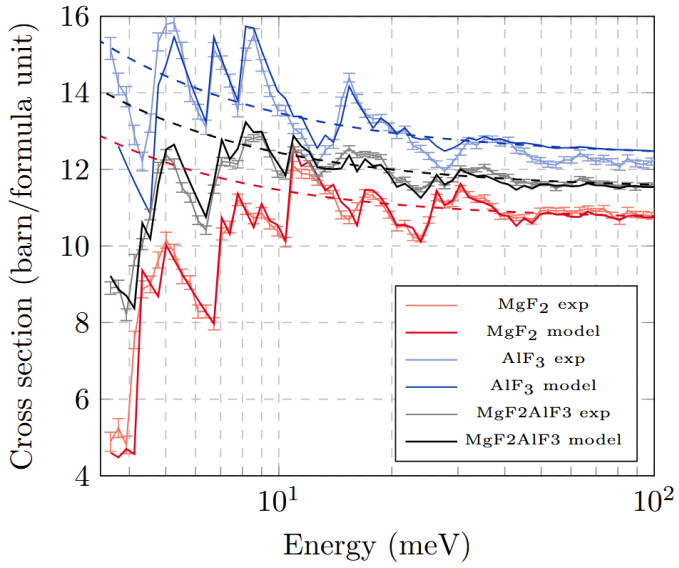


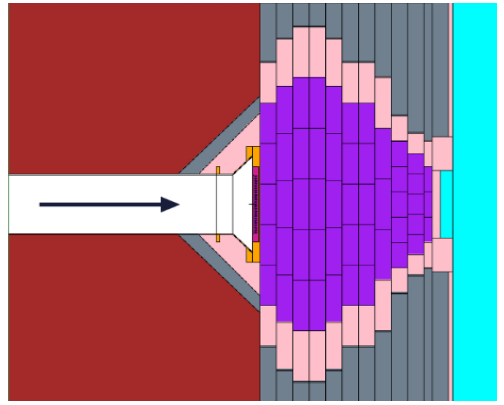
-Simoni, M., Minniti, T., Senesi, R., & Romanelli, G. (2023). Molecular specificity in neutron imaging: the case of hydrogen adsorption in metal organic frameworks. Phys. Chem. Chem. Phys. 25, 30821-30831.

Experimental validation of the scattering libraries for thermal neutron transport within moderators for BNCT



Here, Bragg edges were modelled using the CIF files obtained within the analysis of the concurrent diffraction measurements.





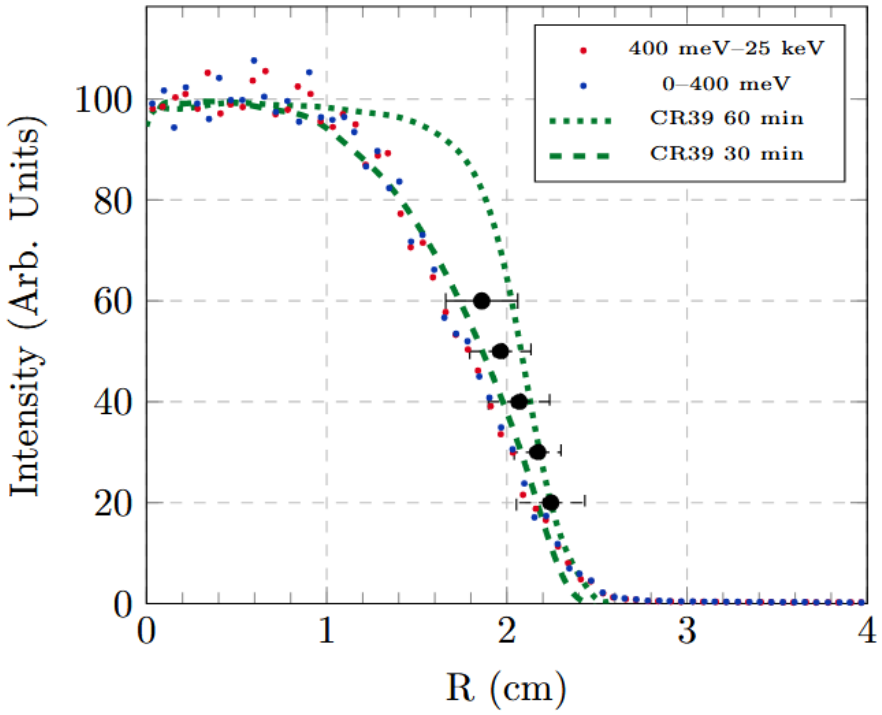
Small angle neutron scattering was approximated by representing the crystals as homogeneous spheres of radius R, and assuming the scattering processes as both elastic and coherent.

Accepted: Simoni, M., Fatemi, S., Airoldi, L., Bortolussi, S., Gaboardi, M., Krzystyniak, M., Marsicano, A., Minniti, T., Porras, I., Postuma, I., Ramos, R., Senesi, R., Tamburini, U. A., Vercesi, V., & Romanelli, G. (2025). Thermal neutron cross sections of aluminum and magnesium fluorides and quantum kinetic energy of fluorine. Journal of Physical Chemistry

Boron Neutron Capture Therapy research from radiobiology to neutron beam design: A truly interdisciplinary voyage. Bortolussi S. et al, relazione su invito, SIF 2025.

Use of CR-39 Dosimeters for the Imaging of Neutron Beam Profiles.

CR-39 were employed for the beam shape characterization of the VESUVIO spectrometer



Through comparison with irradiation with 14 MeV neutrons at the NILE Facility at ISIS, and transport simulations, we show that the majority of defects on the etched surface of the dosimeters irradiated on VESUVIO were induced by neutrons with energies between 100 keV and 10 MeV.

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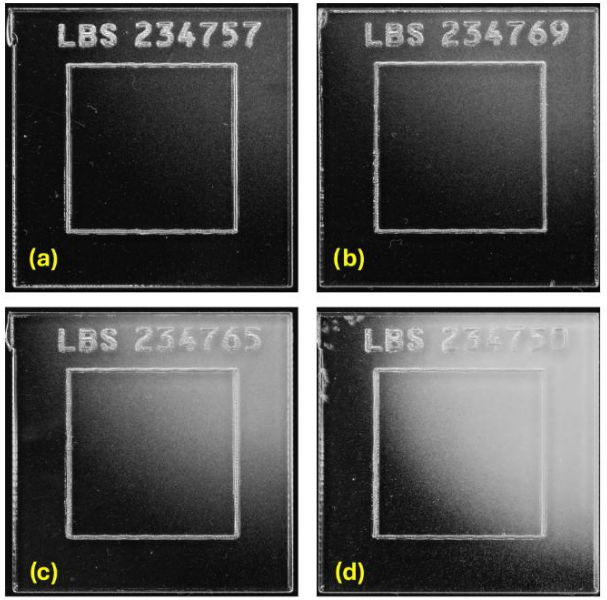
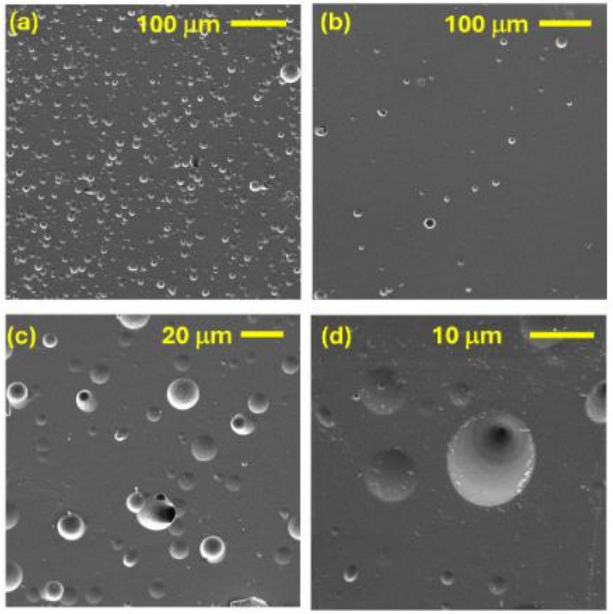
Fisica Sanitaria
Dosimetria





Simoni, M., Baldassarre, L., Cazzaniga, C., Fazi, L., Gaboardi, M., Gemmiti, L., Kastriotou, M., Krzystyniak, M., Marsicano, A., Martellucci, M., Minniti, T., Prioriello, A., Senesi, R., Suteica, V., & Romanelli, G. (2025). Use of CR-39 Dosimeters for the Imaging of Neutron Beam Profiles in the 100 keV–10 MeV Energy Range. Sensors, 25(18), 5865. https://doi.org/10.3390/s25185865

CONFERENCES

Oral presentation | 111° Congresso Nazionale SIF (23/09/2025)

- “Recent developments in measurement and modelling of thermal neutron cross-sections of hydrated amino acids” Authors: Castellani M., Simoni M., Notari S., Gambardella G., Krzystyniak M., Minicozzi V., Stellato F., Bocedi A., Senesi R., Romanelli G.

Oral presentation | Nuclear data 2025 (26/06/2025)

- “Recent developments in measurement and modelling of thermal neutron cross sections of hydrogen-rich materials” Authors: M. Simoni, C. Andreani, R. Senesi, T. Guaragnone, E. Fratini, M. Krzystyniak and G. Romanelli

Poster | *Nuclear data 2025 (*24/06/2025*)*

- “Rotational and magnetic contributions to the thermal neutron cross section of air” Authors: G. Romanelli, Margherita Simoni, M. Krzystyniak, A. Marsicano, T. Giovannini, R. Senesi

Oral presentation | 110° Congresso Nazionale SIF (13/09/2024)

- “The thermal neutron cross-sections of air: The contribution of molecular rotations.” Authors: M. Simoni, R. Senesi, G. Romanelli

Poster | IMAGING 2023 (27/09/2023)

- “Neutron imaging for the catalyzed hydrogen conversion in metal organic frameworks” Authors: M. Simoni, C. Andreani, R. Senesi, G. Romanelli

Oral presentation | SICC Series 2023 (26/09/2023)

- “Recent developments in measurement and modelling of thermal neutron cross sections for radiation shielding and moderation” Authors: M. Simoni, C. Andreani, R. Senesi, G. Romanelli

Oral presentation | 109° Congresso Nazionale SIF (15/09/2023)

- “Neutron imaging for the catalyzed hydrogen conversion in metal organic frameworks” Authors: M. Simoni, C. Andreani, R. Senesi, G. Romanelli

PUBLICATIONS

- Accepted: Simoni, M., Fatemi, S., Airoldi, L., Bortolussi, S., Gaboardi, M., Krzystyniak, M., Marsicano, A., Minniti, T., Porras, I., Postuma, I., Ramos, R., Senesi, R., Tamburini, U. A., Vercesi, V., & Romanelli, G. (2025). Thermal neutron cross sections of aluminum and magnesium fluorides and quantum kinetic energy of fluorine. Journal of Physical Chemistry.
- Simoni, M., Baldassarre, L., Cazzaniga, C., Fazi, L., Gaboardi, M., Gemmiti, L., Kastriotou, M., Krzystyniak, M., Marsicano, A., Martellucci, M., Minniti, T., Prioriello, A., Senesi, R., Suteica, V., & Romanelli, G. (2025). Use of CR-39 Dosimeters for the Imaging of Neutron Beam Profiles in the 100 keV–10 MeV Energy Range. Sensors, 25(18), 5865. https://doi.org/10.3390/s25185865
- Simoni, M., Andreani, C., Fazi L., Prioriello A., Fratini E., Guaragnone T., Krzystyniak M., Senesi, R. & Romanelli, G. (2024). Thermal cross section of poly(2-hydroxyethyl methacrylate) hydrogels for neutron dose calculation. EPJ Plus.
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- Romanelli, G., Simoni, M., Preziosi, E., Damian, J., Andreani, C., & Senesi, R. (2023). Neutron thermal cross sections of 3D-printing organic polymers using the Average Functional Group Approximation. EPJ Web of Conferences, 284, 17010.
- Di Lisio, V., Braunewell, B., Macia-Castello, C., Simoni, M., Senesi, R., Fernandez-Alonso, F., & Cangialosi, D. (2023). Fast scanning calorimetry on volatile carbon-based materials. Thermochimica Acta, 719, 179414.

AWARDS

Premio SIF-SoNS Neutrons-Matter 2025

Thank you

Science and Technology Facilities Council

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