TOR VERGATA
UNIVERSITÀ DEGLI STUDI DI ROMA

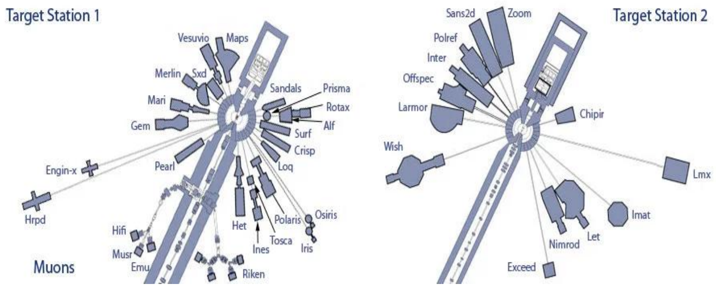
Rotational and magnetic contributions to the thermal neutron cross section of air

Margherita Simoni[1], Felix Fernandez-Alonso[2,3,4], Tommaso Giovannini[1], Matthew Krzystyniak[5], Jose Ignacio Marquez-Damian[6], Anna Marsicano[5], Marco Martellucci[1], Triestino Minniti[1], Roberto Senesi[1,7], Matteo Sorbara[1] and Giovanni Romanelli[1,5*]

[1]*Physics Department, Università degli Studi di Roma Tor Vergata, via della Ricerca Scientifica 1, 00133, Roma, Italy*
[2]*Centro de Fìsica de Materiales (CFM-MPC), CSIC-UPV/EHU, Paseo de Manuel Lardizabal 5, Donostia, 20018, Gipuzkoa, Spain*
[3]*Donostia International Physics Center (DIPC),Paseo de Manuel Lardizabal 4, 20018 Donostia - San Sebastian, Spain*
[4]*IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 5, 48009 Bilbao, Spain*
[5]*ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Chilton OX110QX, United Kingdom*
[6]*European Spallation Source, ESS ERIC, Partikelgatan 2, 224 84 Lund, Sweden*
[7]*Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche, Via del Fosso del Cavaliere, 100, Rome, 00133, Italy*

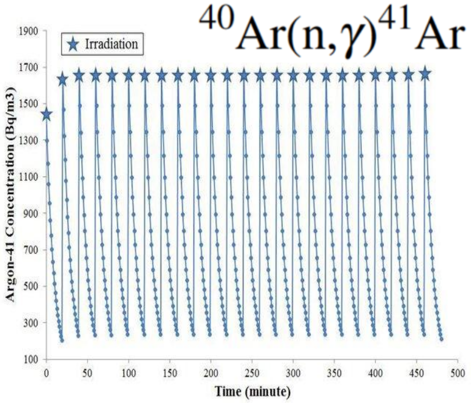
Motivation

Thermal neutron cross sections are essential for **Monte Carlo** transport simulations used to guide device design and operation. Air presence is often approximated in the design of:

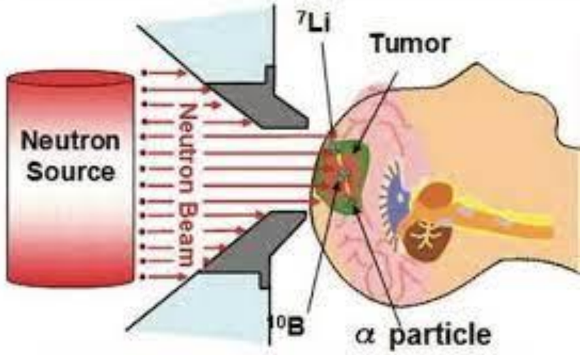


Design and operation of neutron facilities

LINAC for radiotherapy



Boron neutron capture therapy



When operating a LINAC for radiotherapy, **ventilation systems** are used to dilute and remove activated air

Latifah, R & Bunawas, & Noor, Johan. (2018). Journal of Physics: Conference Series

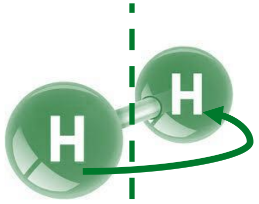
Discrepancies with experimental results are often attributed to uncertainties of **air humidity**, however, **molecular motion is not considered!**

e.g.: J Appl Crystallogr. 2015 Jun 27;48(Pt 4):1055-1071.

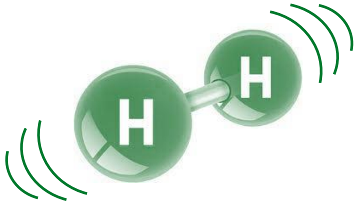
Young and Koppel model

The cross section of diatomic molecules such as N_2 and O_2 depends on multiple degrees of freedom and is not well approximated by a **free gas model**. Diatomic molecules can:

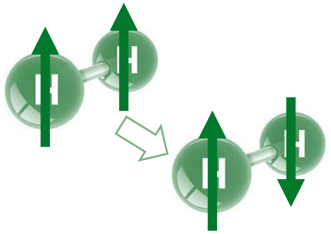
rotate about their centre of mass



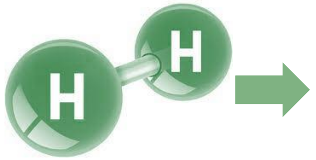
vibrate along their axis



flip their spin

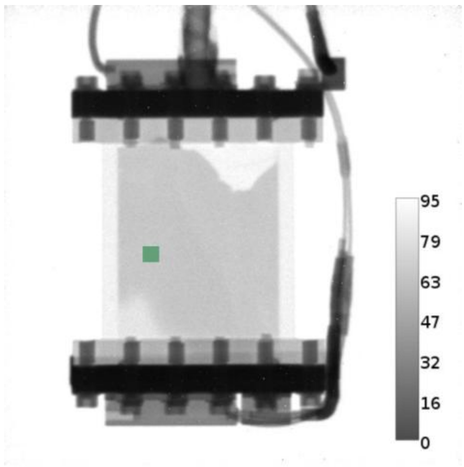


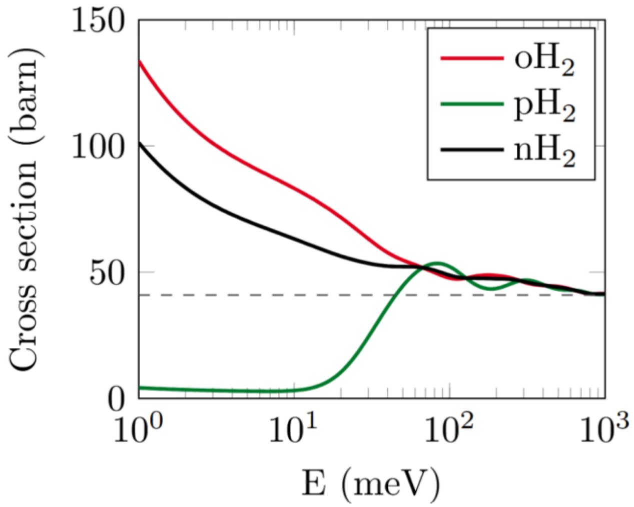
and move in space



The cross section of diatomic molecules can be calculated using the **Young and Koppel model**

J. A. Young and J. U. Koppel. Slow neutron scattering by molecular hydrogen and deuterium. *Phys. Rev.,* 135:A603–A611, Aug 1964.





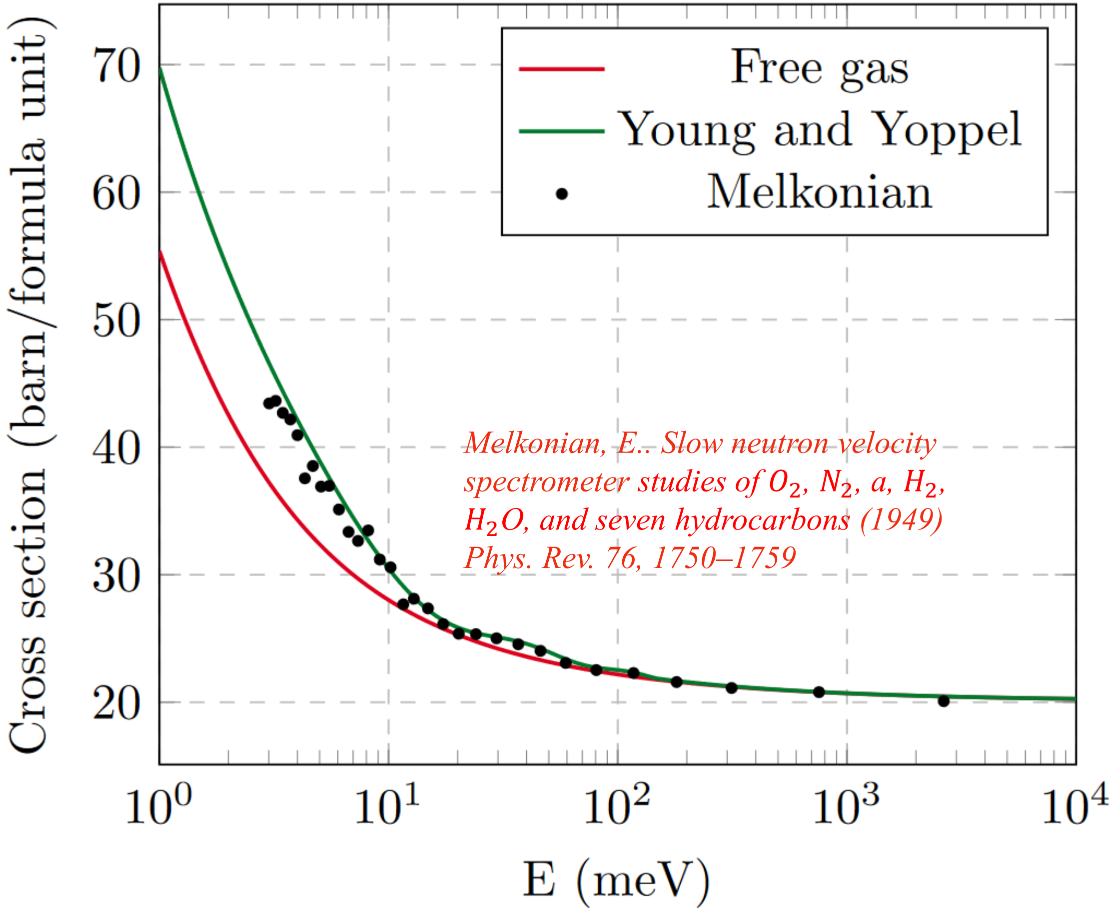
-Simoni, M., Minniti, T., Senesi, R., & Romanelli, G. (2023). Molecular specificity in neutron imaging: the case of hydrogen adsorption in metal organic frameworks. Phys. Chem. Chem. Phys. 25, 30821-30831.

Thermal neutron cross section of N_2

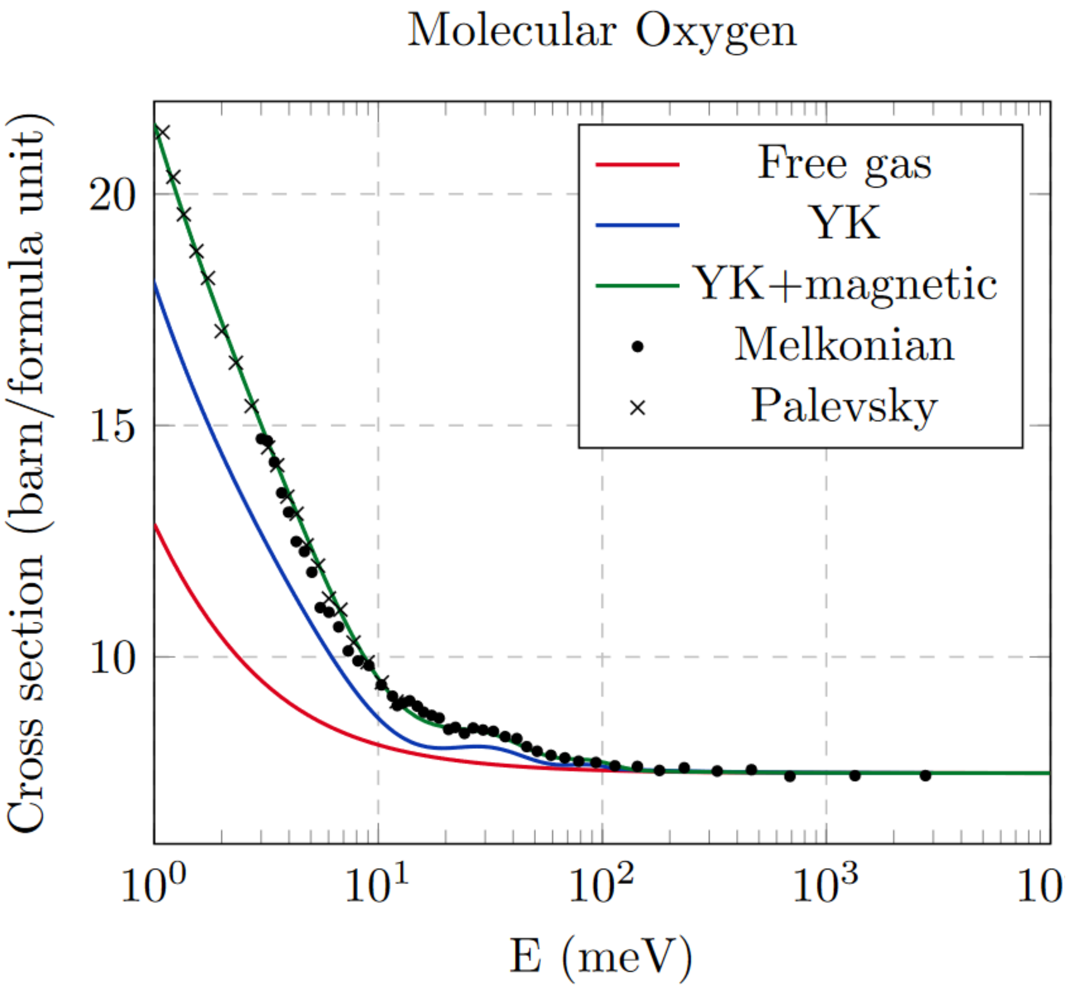
We performed the calculation of thermal neutron cross section of diatomic molecules that are abundant in air

Molecule	Total Sym.	I	J	Electronic ground state
N_2	S = S×S×S	2 (ortho)	0,2,...	$^1\Sigma_g^+$
	S = A×A×S	1 (para)	1,3,...	
	S = S×S×S	0 (ortho)	0,2,...	
O_2	S = S×A×A	0 (ortho)	1,3,...	$^3\Sigma_g^-$

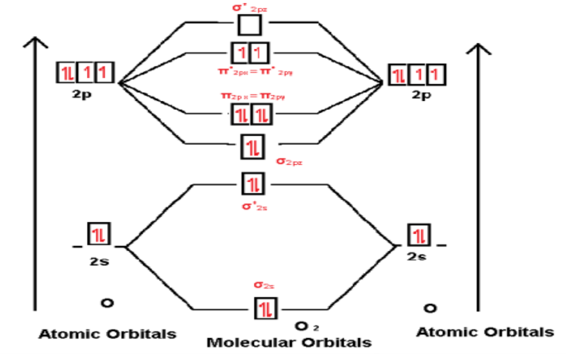
Neutron scattering cross section was estimated using **Young and Koppel model**, and compared to the free gas model and to experimental data from 1955.



Thermal neutron cross section of O_2



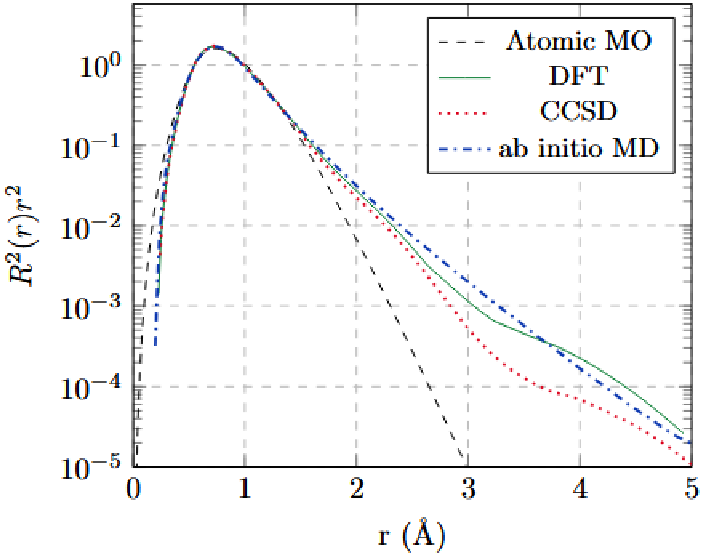
Young and Koppel model was not enough to reproduce O_2 cross section: Its paramagnetic behaviour need to be considered.

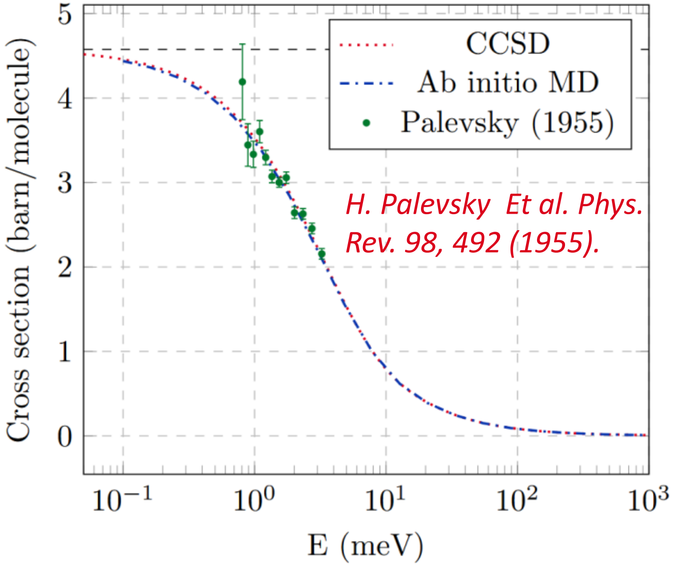


$$\frac{d\sigma_s}{d\Omega} = \frac{2}{3}\left(\frac{\mu}{m_n}\right)^2 \gamma^2 r_0^2 S(S+1) e^{-2W(Q)} f^2(Q)$$

$$f(Q) = \int_0^\infty j_o(Qr) r^2 R^2(r) dr$$

W. H. Kleiner, "Magnetic scattering of slow neutrons from o2 gas," Phys. Rev. 97, 411–418 (1955).





H. Palevsky Et al. Phys. Rev. 98, 492 (1955).

Thermal neutron cross section of air

Air composition was approximated as:

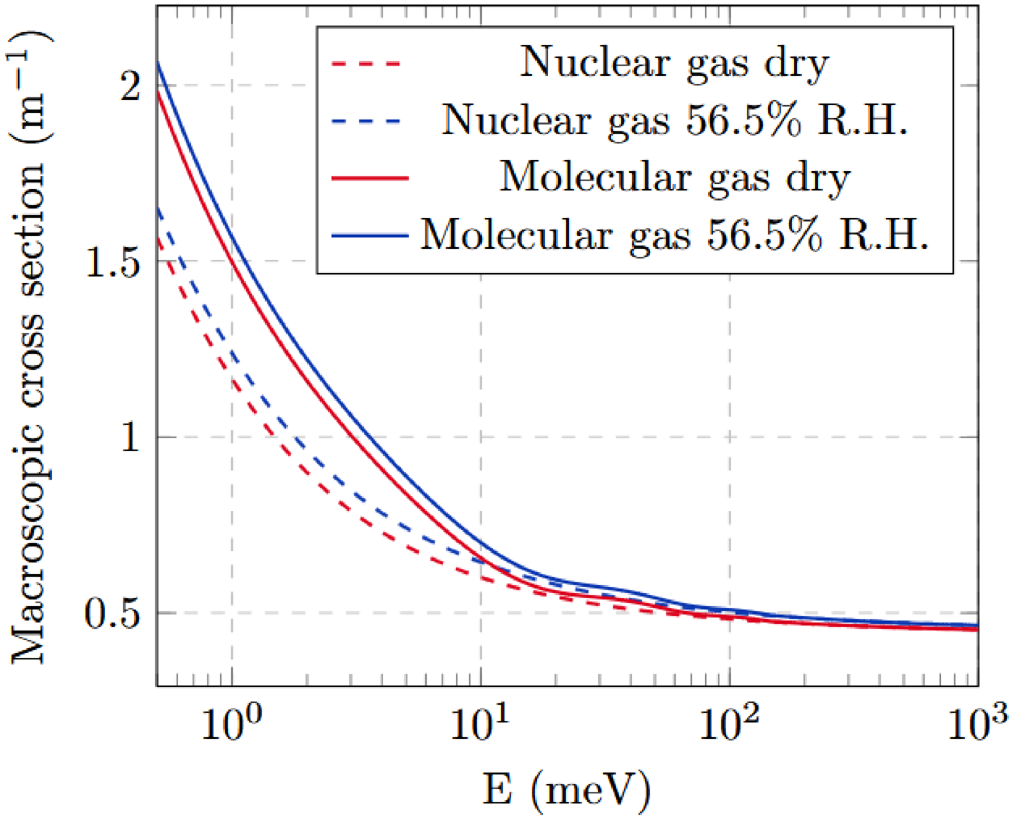
Isotope	mol% in dry air	mol% in hydrated air	Reaction	Absorption XS (barn)
^{14}N	0.7848	0.7696	$^{14}N(n,\gamma)^{15}N$ $^{14}N(n,p)^{14}C$	0.075 1.84
^{16}O	0.2105	0.2064 in O_2 0.0065 in H_2O	$^{16}O(n,\gamma)^{17}O$	0.0001
^{40}Ar	0.0047	0.0046	$^{40}Ar(n,\gamma)^{41}Ar$	0.66
^{1}H	0	0.0129	$^{1}H(n,\gamma)^{2}H$	0.3326

Water was approximated as liquid, with the use of the CAB model:

J. Màrquez-Damiàn, J. Granada, D. Malaspina, CAB models for water: A new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format. Ann. Nucl. Energy 65, 280–289 (2014)

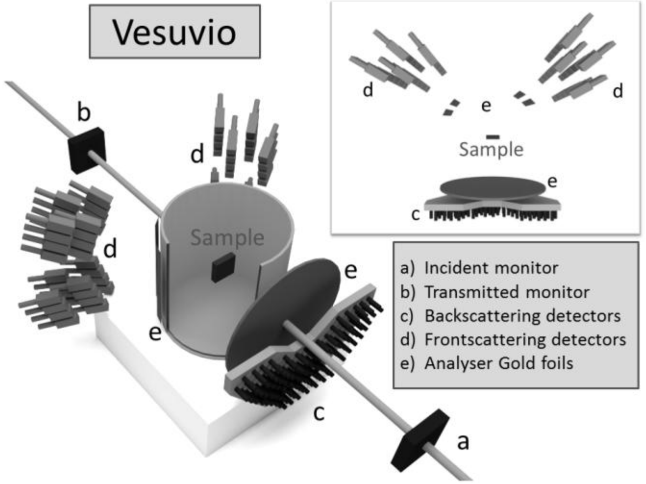
- Mole fraction of water vapour was calculated according to appendix A.1 of https://www.nist.gov/system/files/documents/calibrations/CIPM-2007.pdf

Parameter	Value
Air Density	0.001225 g/cm^3
Humidity	56.5 %
Pressure	1.013×10^5 Pa
Temperature	293.6 K



We found that air cross section is strongly affected by molecular rotations!

Measuring neutron cross section of air

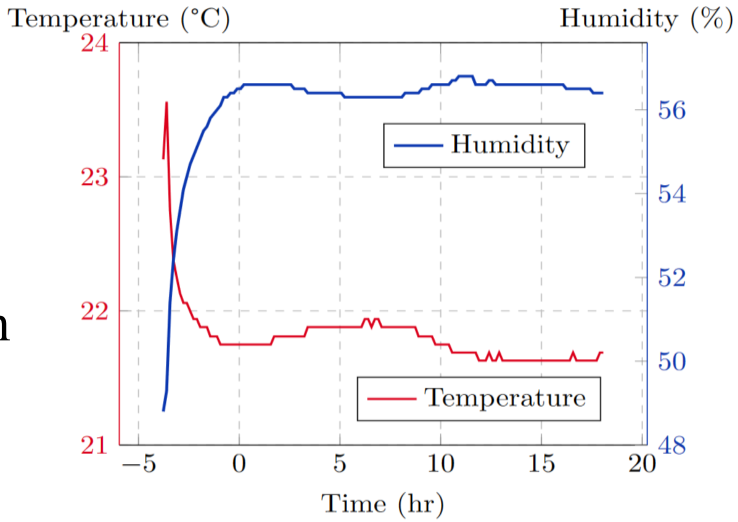


VESUVIO spectrometer was employed to perform **transmission measurements**

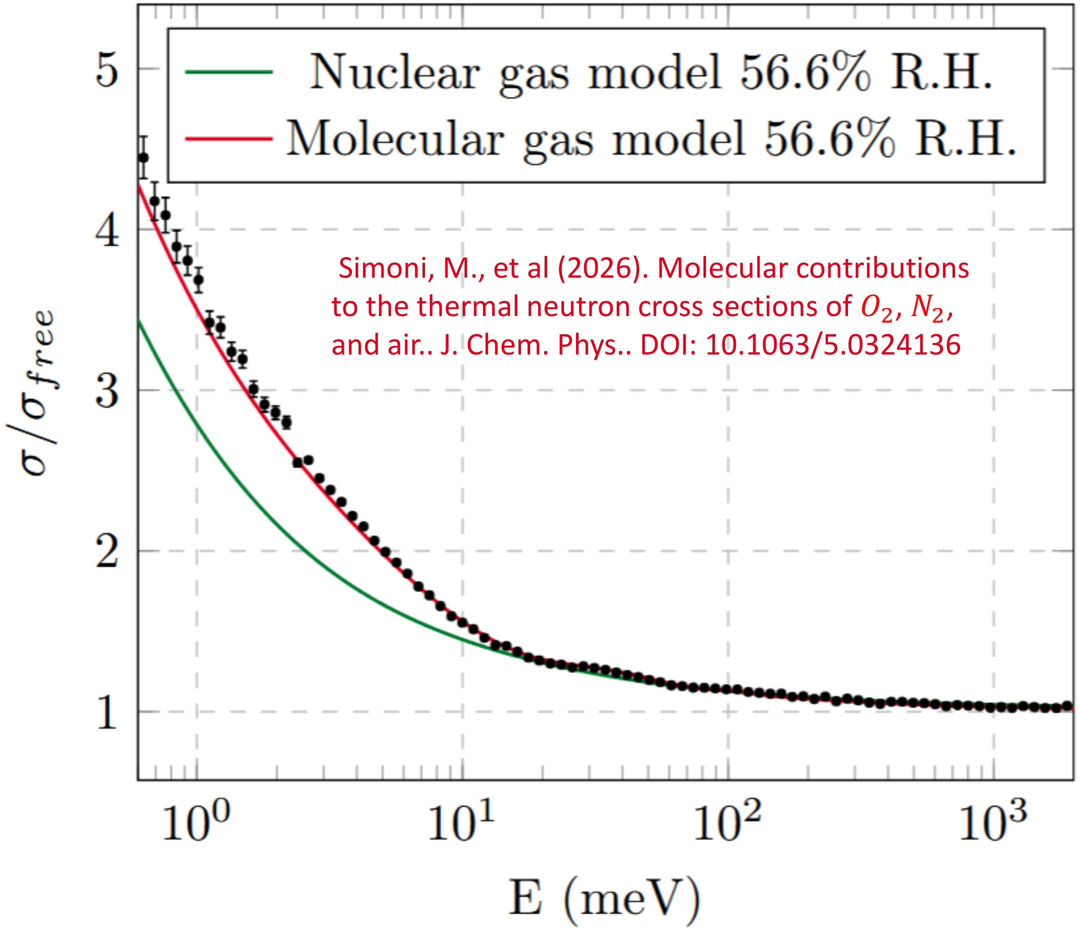
Science and Technology Facilities Council

ISIS Neutron and Muon Source

- Good geometry was checked through Monte Carlo simulation



Free gas and **molecular gas models** are compared to **experimental data**:

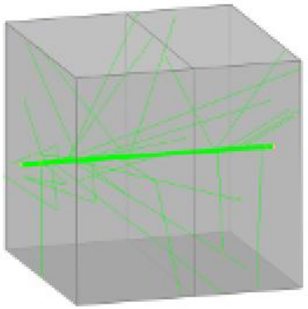


Simoni, M., et al (2026). Molecular contributions to the thermal neutron cross sections of O_2, N_2, and air.. J. Chem. Phys.. DOI: 10.1063/5.0324136

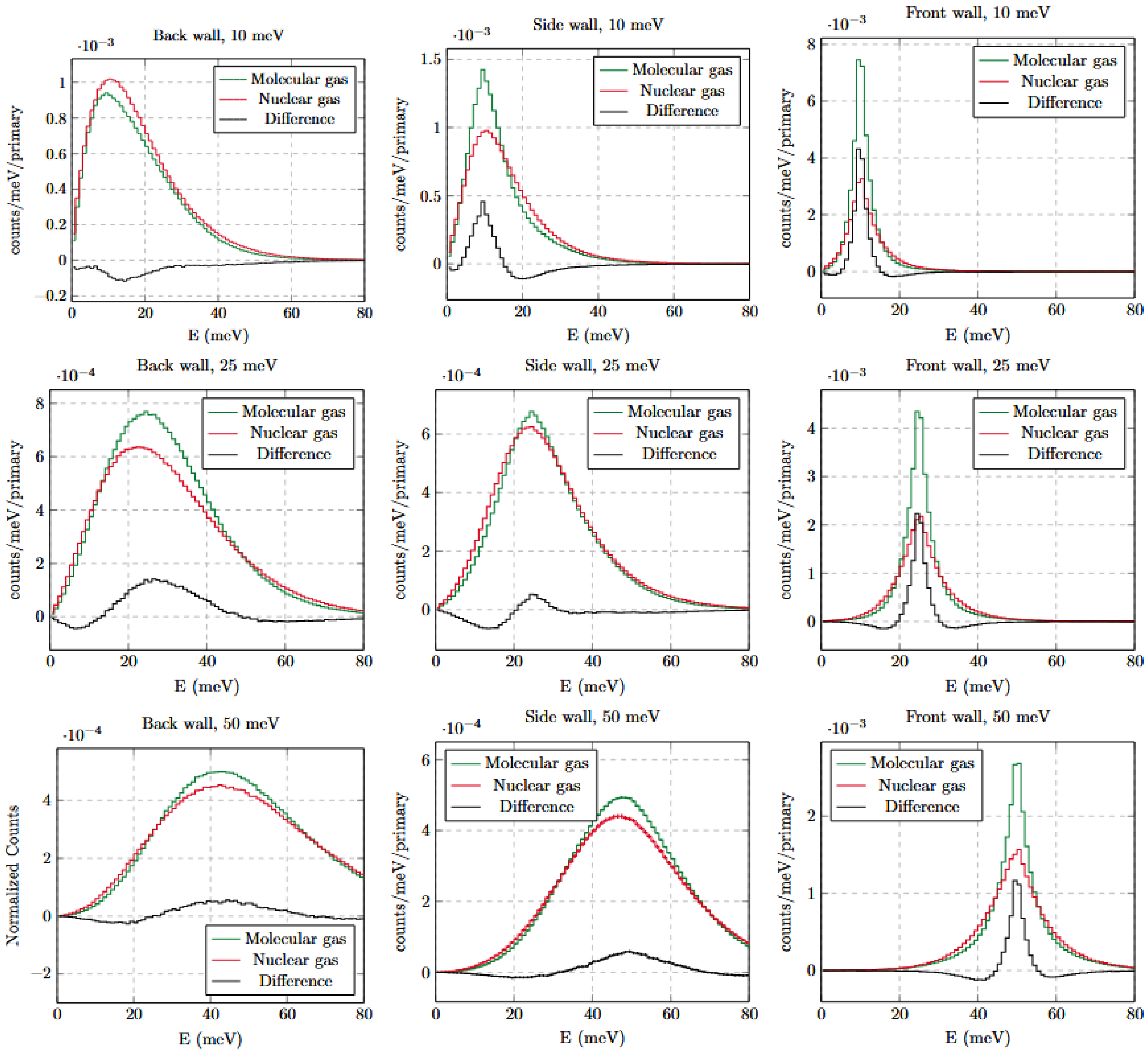
Monte Carlo transport simulations

Geant 4 transport simulations with the use of the **Ncrystal toolkit**

X. Cai, T. Kittelmann, **Ncrystal**: A library for thermal neutron transport. Comput. Phys. Commun. 246, 106851 (2020)



The room is of 3×3×3 m3. The incident neutron beam (thick green line) is oriented along the z axis.



Conclusions and outlook

- The Young and Koppel model, together with the paramagnetic model, proved to better estimate the total cross section of air at a given humidity percentage.
- We plan to improve the model by including gaseous water, instead of liquid.
- We plan to make the model easily accessible, together with the models for homonuclear diatomic molecules
- The model was recently published in → Simoni, M., et al (2026). Molecular contributions to the thermal neutron cross sections of O2, N2, and air.. J. Chem. Phys.. DOI: 10.1063/5.0324136

Thank you for your time!