TOWARDS THE DEVELOPMENT OF A VERY COLD NEUTRON SOURCE

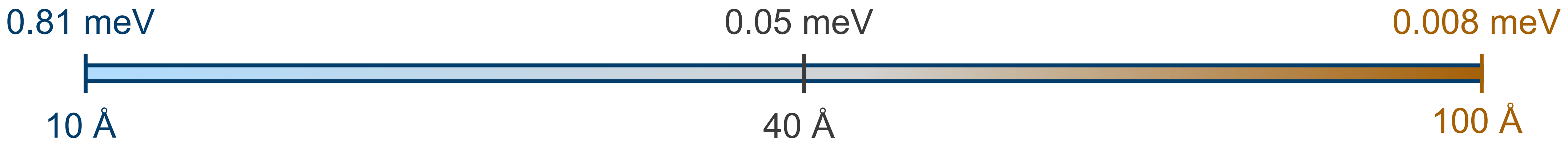
FOR THE HIGH BRILLIANCE NEUTRON SOURCE (HBS)

14.02.2024 I DALINI D. MAHARAJ

VERY COLD NEUTRONS

Range of very cold neutrons

- 10 - 100 Å



- Cannot produce reasonable intensities from conventional cold sources!!
  - Neutron spectra follow a Maxwellian shape
  - For long neutron wavelengths (low energies) spectrums falls off as λ^{-5}

POTENTIAL FOR VERY COLD NEUTRONS

Proceedings of the Workshop on Applications of a Very Cold Neutron Source

ARGONNE NATIONAL LABORATORY

ANL-05/42

Proceedings of the Workshop on Applications of a Very Cold Neutron Source

August 21-24, 2005

prepared by
Intense Pulsed Neutron Source Division
Argonne National Laboratory

- Access to longer length and time scales – large biological structures on the nanoscale
- Refracting power ≈ λ^2

  => Application of optical methods to control neutron beams

POTENTIAL FOR VERY COLD NEUTRONS

	Resolution (at fixed geometry)	Intensity (at fixed resolution)
SANS	λ^{-1}	λ^{0}
Reflectometry	λ^{-1}	λ^{2}(?)
TOF-INS	λ^{-3}	λ^{2}
NSE	λ^{-3}	λ^{2} - λ^{4}

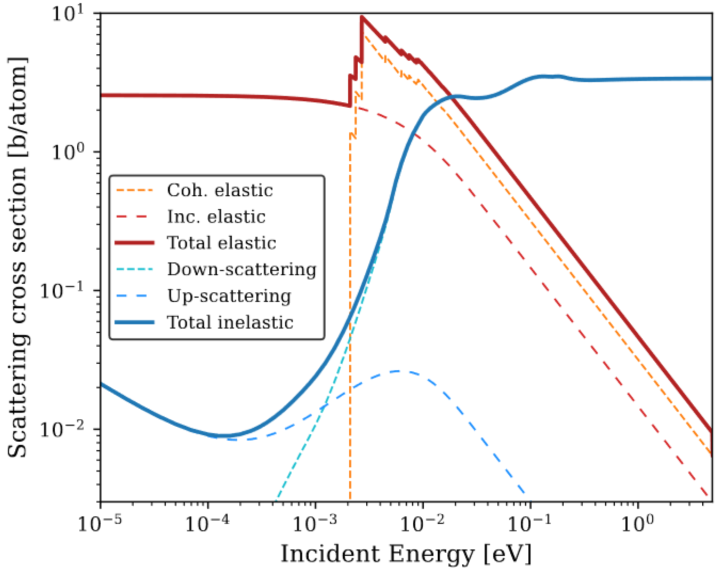
[1] J.M Carpenter and B.J. Micklich, ANL (05/42) (2005).

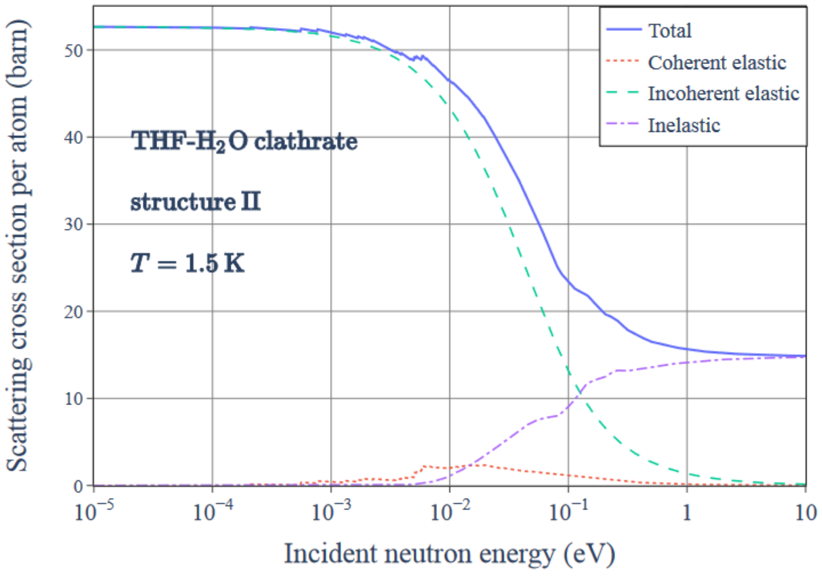
- Access to longer length and time scales – large biological structures on the nanoscale
- Refracting power ≈ λ^2

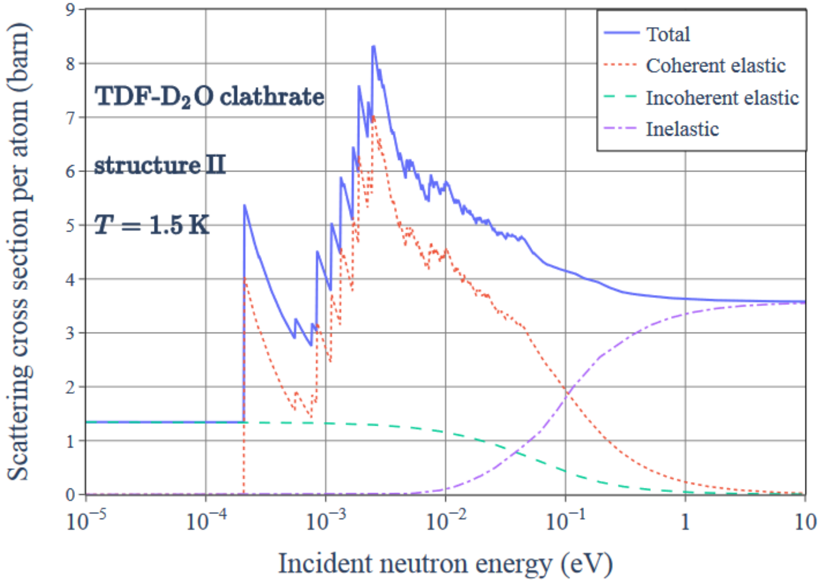
  => Application of optical methods to control neutron beams
- Predicted gains in improvement in instrument performance

WHY NOW?

Previously, lack of available neutron cross sections at low temperatures for moderators of interest







[2] L. Zanini, arXiv:2309.17333v3 [physics.ins-det] (2023).

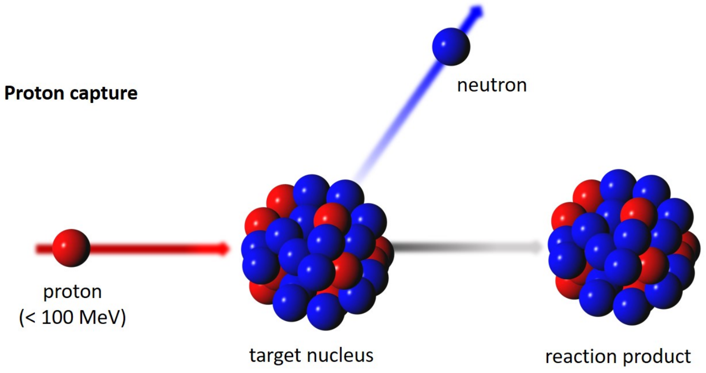
[3] S. Xu, EPJ Web of Conferences **286** 06003 (2023)

- Neutron scattering kernels developed through the HighNESS project for many candidate moderator and reflector materials
- Opportunity to explore VCN development for HBS

SPALLATION VS HI-CANS

Comparison of Source Optimization Objectives

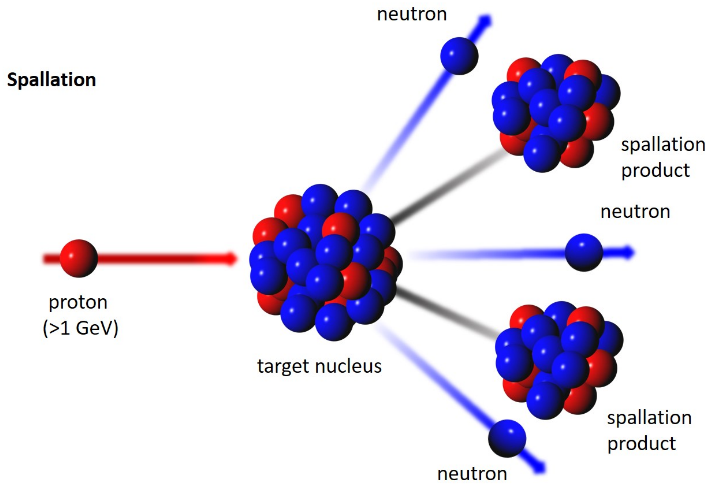
Hi-CANS
~ 0.02 n/p



Optimize brilliance

$$B = \frac{d}{A\,\Omega(1\%\Delta\lambda/\lambda)\Delta t}$$

Spallation
~ 27 n/p



Optimize overall time-integrated intensity

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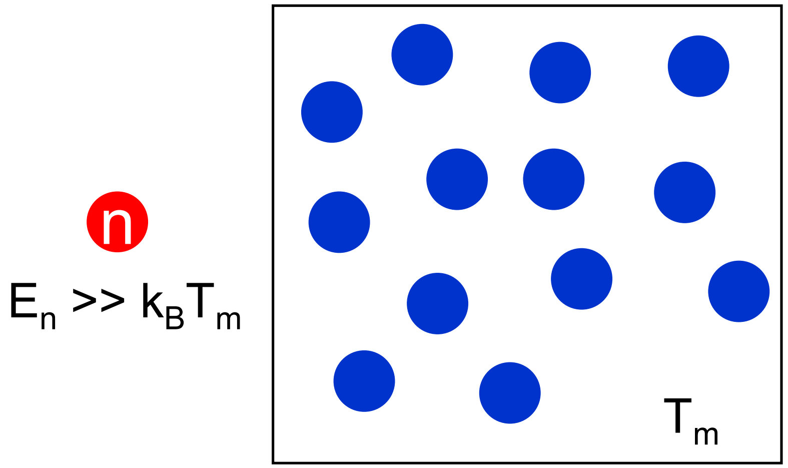
MODERATION OF NEUTRONS

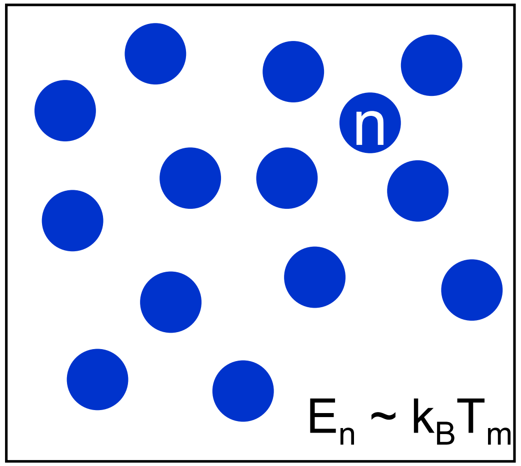
Moderating properties of material

- Coupling strength to the neutron field via cross section
- Excitation spectrum of material e.g. phonons



BUT phonon cross section for neutron with $E < k_B T_D$

$$\left(\frac{E}{k_b T_D}\right)^3$$



Very cold moderation requires low, dispersion-free “quantum” excitation modes

- Einstein modes – displacement of confined molecules
- Molecular rotations
- Librations
- Paramagnetic excitations

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CANDIDATE VERY COLD MODERATORS

Solid D_2

- Rotational modes and vibrational modes
- Operates at 5 K

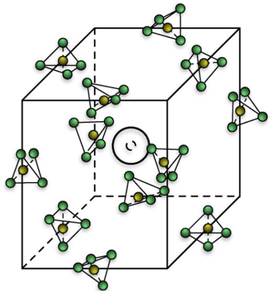
Pros:

- Low neutron absorption
- High scattering cross section

Cons

- Long neutron path length dilutes neutron cloud

Methane (in phase II)



- Phase II below 20.4 K
- Free rotor at O_h site

Pros:

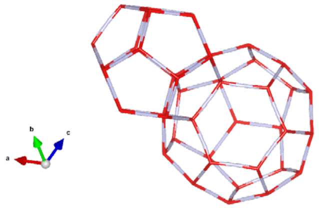
- Very good moderator due to high density of hydrogen atoms

Cons:

- Radiolysis, or radical formation needs to be managed

Clathrates (THF, methane)

- Cages host guest molecules including
  - O_2 (ZF – 0.4meV)
  - CH_4
  - THF



Pros:

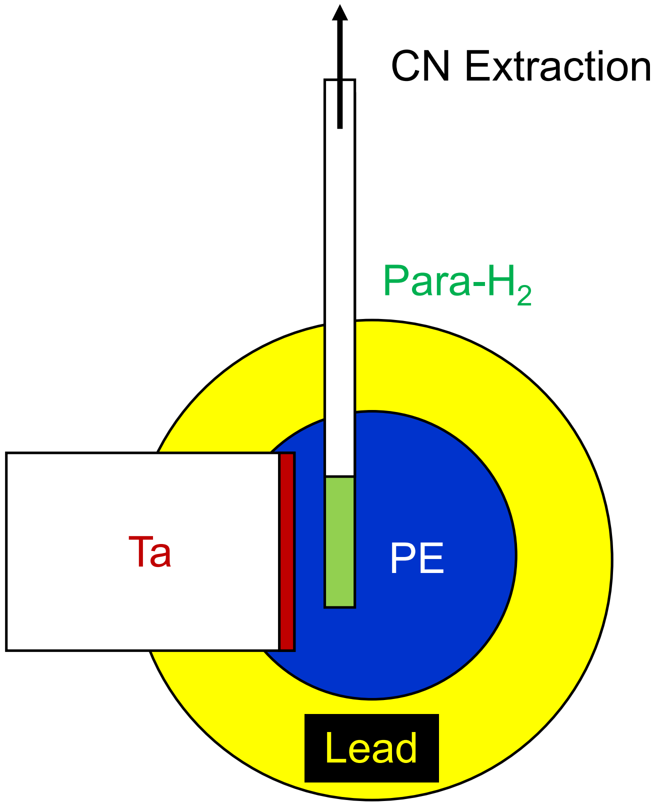
- High albedo for CN

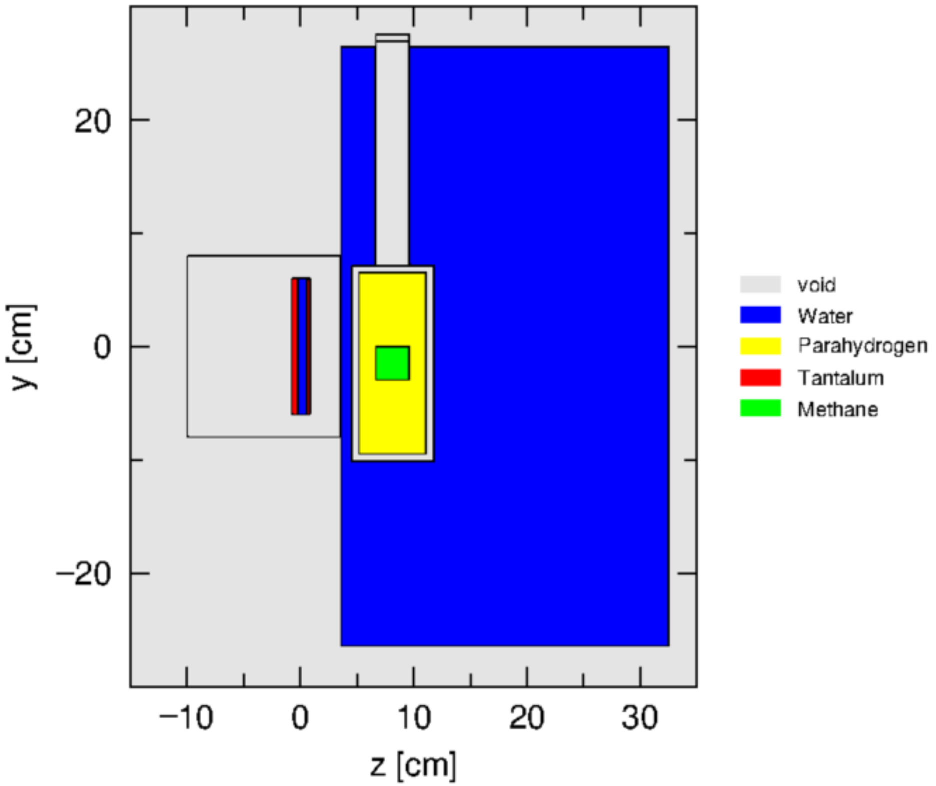
Cons:

- Operation at 2.4 K

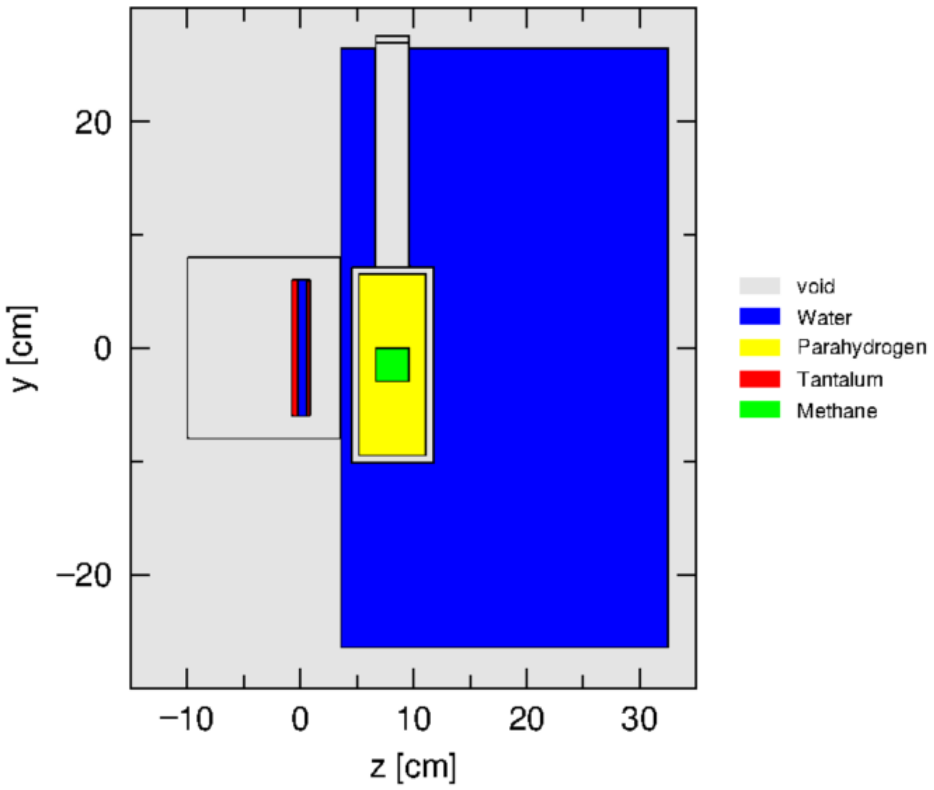
HIGH BRILLIANCE MODERATOR DESIGN

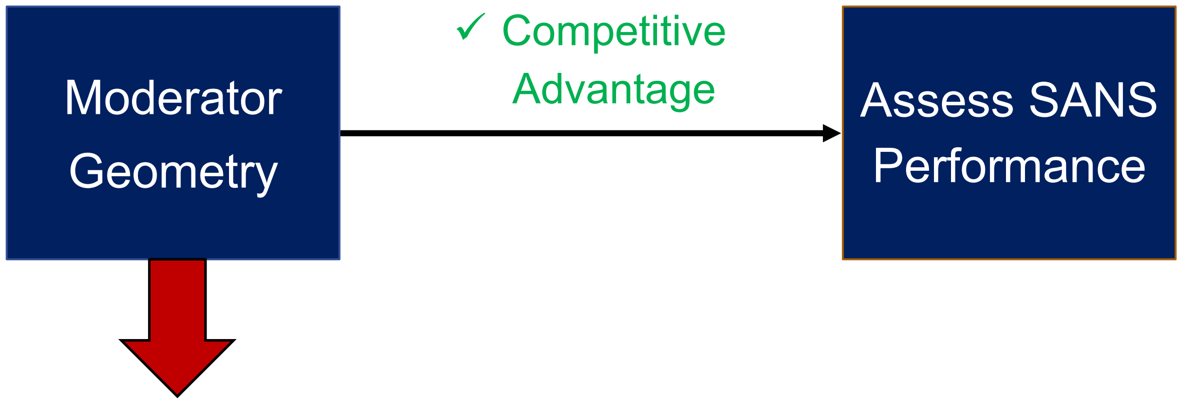
Compact 2D Cold Parahydrogen Moderator





WORKFLOW IN PHITS





Demonstrate superior performance to 2D parahydrogen beyond 10 Å

$$B = \frac{d}{A\,\Omega(1\%\Delta\lambda/\lambda)\Delta\,t}$$

Show gains in intensity beyond 10 Å; slower fall-off in intensity beyond 10 Å than λ^{-5} for conventional cold moderators

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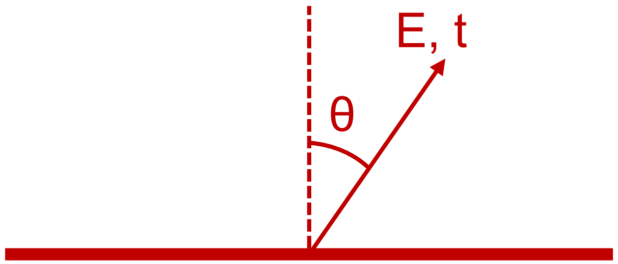
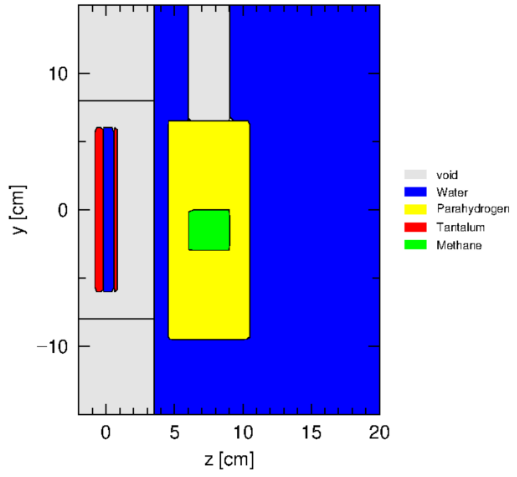
CALCULATED QUANTITIES IN PHITS

Surface Tally

- Define detector at exit of channel and tally neutrons in energy, time, angular crossing bins
- Can estimate brilliance directly from this method

$$B = \frac{d}{A\,\Omega(1\%\Delta\lambda/\lambda)\Delta\,t}$$





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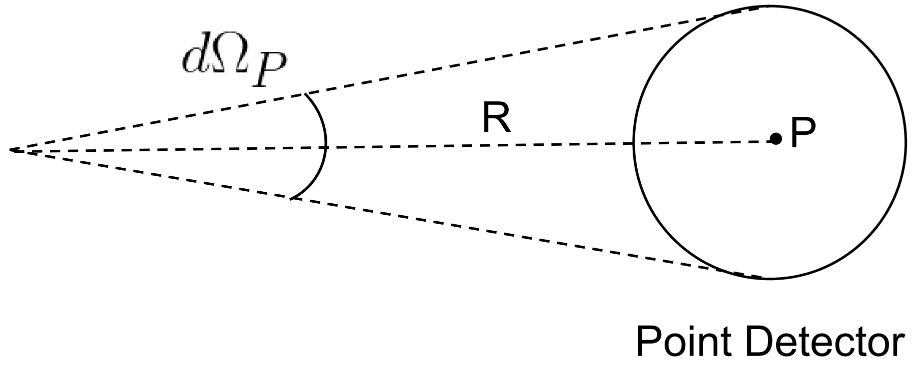
CALCULATED QUANTITIES IN PHITS

Point Tally

- Deterministically estimate of the flux contribution due to every source or collision event at a point,
  - Scattering probability
  - *T*, transmission probability for no interaction between event and detector points

$$T = \exp\left(-\int_0^R \Sigma(s)\mathrm{d}s\right)$$

$$\Phi = w\frac{p(\mu)}{2\pi R^2}\exp\left[-\int_0^R \Sigma(s)\mathrm{d}s\right].$$



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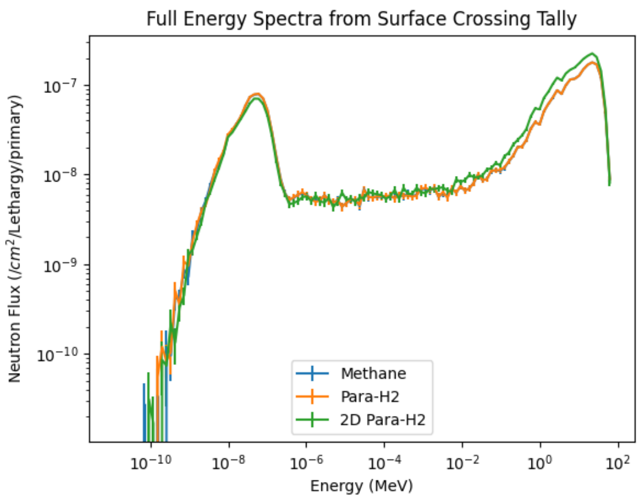
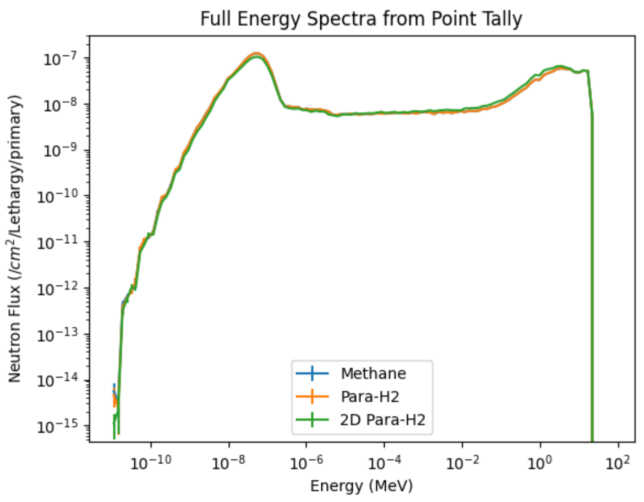
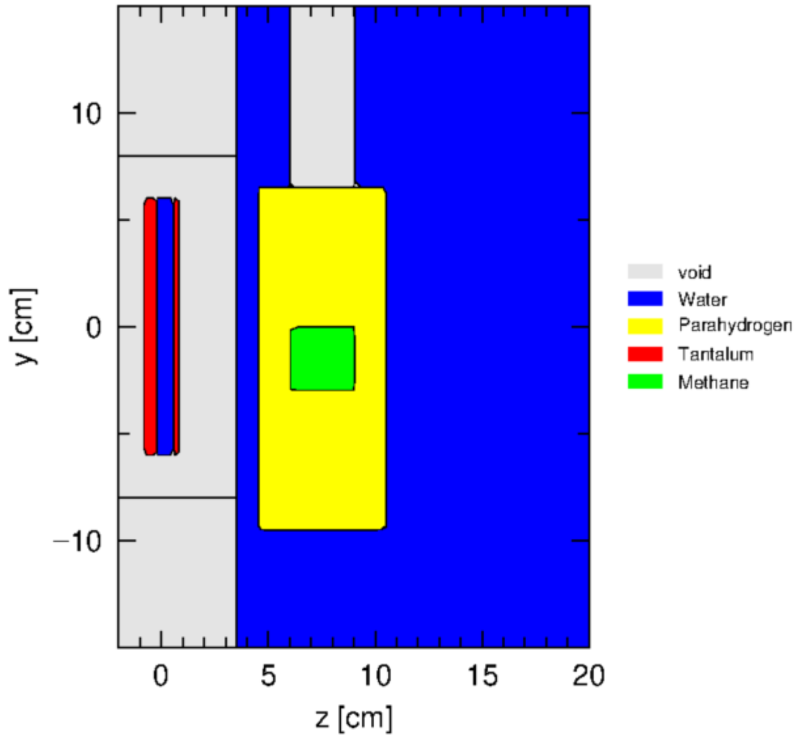
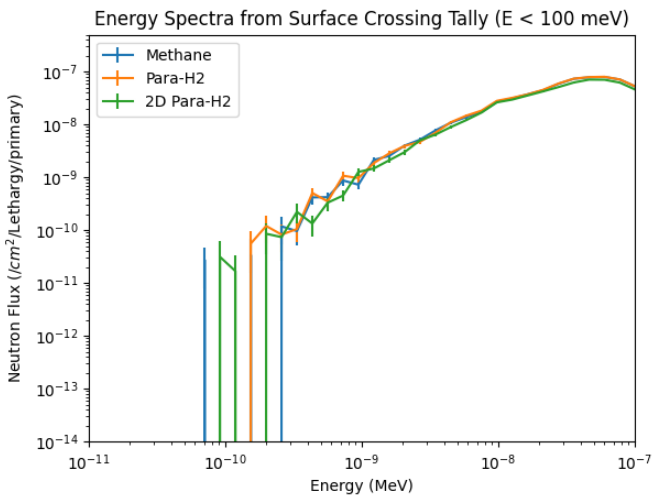
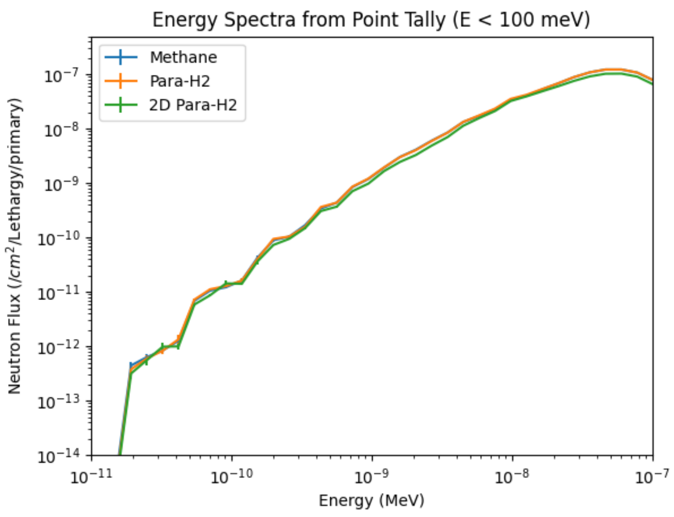
SURFACE CROSSING TALLY VS POINT TALLY











MAJOR CHALLENGES AND CONSIDERATIONS

Computational demands of simulations

Practical considerations

- ➢ Moderating to very cold neutron energies within compact volume
- ➢ Managing heat removal from the moderator
  - Use of aluminum foams to improve thermal conductivity

NEXT STEPS

Computational

- ➢ Implementation of point tally to get first “feel”
- ➢ Accelerate duration for each simulation – use neutron source characteristics of moderator
- ➢ Very high statistics required => demand for raw computation power
  - Apply to JSC for computation time. JUREAP program

Upcoming Secondment

- ➢ Implementation of OpenMC to perform simulations with clathrates
- ➢ Techniques and tools for multi-parameter optimization

HBS Team

JCNS (Jülich Centre for Neutron Science)

J. Baggemann
Th. Brückel
J. Chen
T. Claudio-Weber
T. Cronert (†)
Q. Ding
P.-E. Doege
M. El Barbari
T. Gutberlet
J. Li
K. Lieutenant
Z. Ma
E. Mauerhofer
N. Ophoven
U. Rücker
N. Schmidt
A. Schwab
E. Vezhlev
J. Voigt
P. Zakalek

- Design, verification, instrumentation

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ZEA-1:
Y. Bessler
R. Hanslik
R. Achten
F. Löchte
M. Strothmann

- Engineering

IKP-4:
O. Felden
R. Gebel
A. Lehrach
M. Rimmler
R. Similon

- Nuclear physics

INM-5:
B. Neumaier

- Radio isotopes

net – Nukleare Entsorgung und Techniktransfer, RWTH AACHEN

S. Böhm
R. Nabbi

- Nuclear simul.

TECHNISCHE UNIVERSITÄT DRESDEN

Ch.Haberstroh
M. Klaus
S. Eisenhut
C. Lange

- Liquid H_2, AKR-2

IAP – Institut für Angewandte Physik

H. Podlech
O. Meusel

- Accelerator

GSI / HIM – GSI Helmholtzzentrum für Schwerionenforschung GmbH

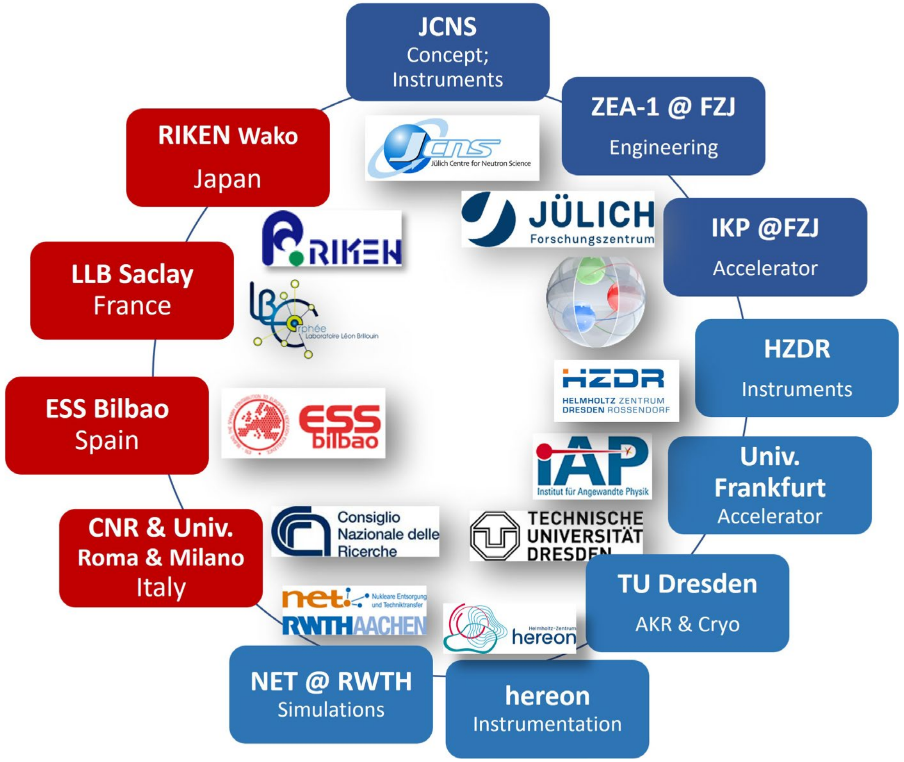
W. Barth

- Accelerator

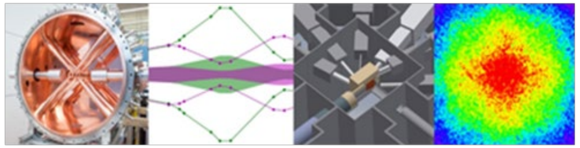
Helmholtz-Zentrum hereon

J. Fenske

- Instrumentation



HBS Innovationpool Project



FB Matter: MML, MT

Federal Ministry of Education and Research

ELENA
European Low Energy accelerator-based Neutron facilities Association

@hbsneutron

https://hbs.fz-juelich.de/

REFERENCES

[1] J.M Carpenter and B.J. Micklich, ANL (05/42) (2025).

[2] L. Zanini, arXiv:2309.17333v3 [physics.ins-det] (2023).

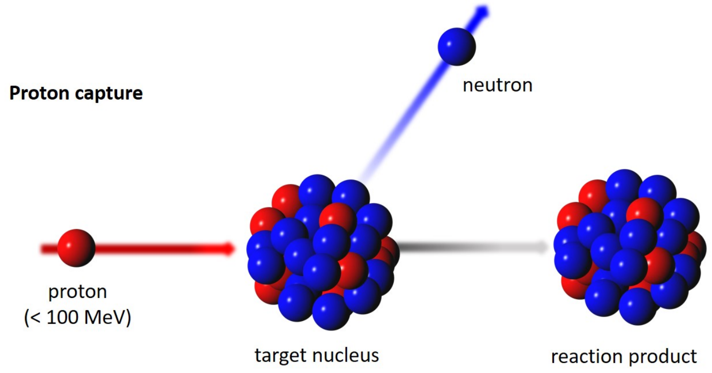
[3] S. Xu, EPJ Web of Conferences **286** 06003 (2023)

HI-CANS

From Neutron Generation to Extraction

Hi-CANS

~ 0.02 n/p



Optimize brilliance

$$B = \frac{d}{A\,\Omega(1\%\Delta\lambda/\lambda)\Delta t}$$

Source and Moderator Features

- Compact moderator design
- High density neutron clouds in moderators

Brightness Optimization

- Selection of suitable materials
- Moderator design tailored to instruments
- Clever use of optics
  - Efficient transfer of neutron phase space

MODERATION OF NEUTRONS

Proceeds via hard scattering from atomic species in moderating medium

Mean logarithmic reduction in neutron energy, ξ

$$\xi = \ln\left(\frac{E_0}{E}\right)$$

Efficiency of a moderator, moderation ratio, MR

$$\mathrm{MR} = \left(\xi \cdot \frac{\Sigma_s}{\Sigma_a}\right)$$

Diffusion length, L

$$L = \left(\frac{D}{\Sigma_a}\right)^{1/2}$$

Neutrons can also excite vibrational modes in solid state materials

$$\sigma_1^0 \sim \left(\frac{m}{M}\right)\left(\frac{E_0}{k\theta_D}\right)^3$$

Parameters for common thermal moderators

	ξ [barn]	MR	L [cm]
Polyethylene (PE)	0.91	86	2.08
D_2O	0.57	5720	141
$H_2O + D_2O$	0.81	110	7.12
Be	0.21	128	18.33

P. Zakalek *et al*, Journal of Neutron Research **23** pp. 185-200 (2021).

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CANDIDATE VERY COLD MODERATORS

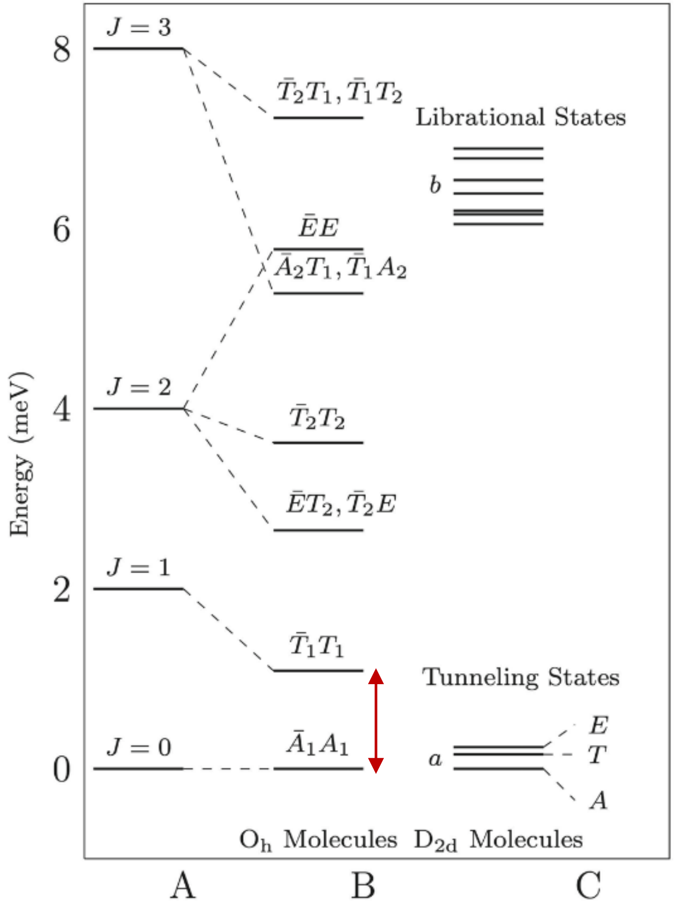
- Solid D_2
- **Methane (in phase II)**
- Clathrates – THF-hydrates, methane hydrate

➢ Transition to phase II below 20.4 K

- Partially orientationally ordered state

Disordered sites - O_h
✓ Weak CEF
✓ No molecular field
Almost free quantum rotor!

Ordered sites - D_{2d}
-Librational modes
-Rotational tunneling



Y. Shin *et al*, Nuc. Ins. Meth Phys Res A **620** pp. 382–390 (2010).

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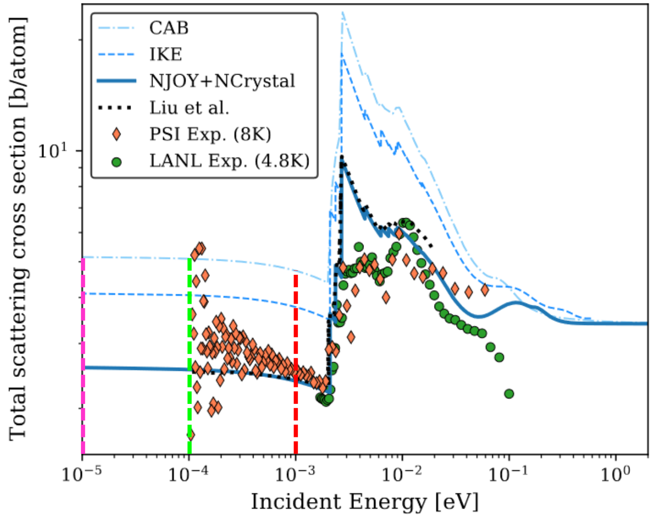
Moderation by: rotational and translational modes (phonons)

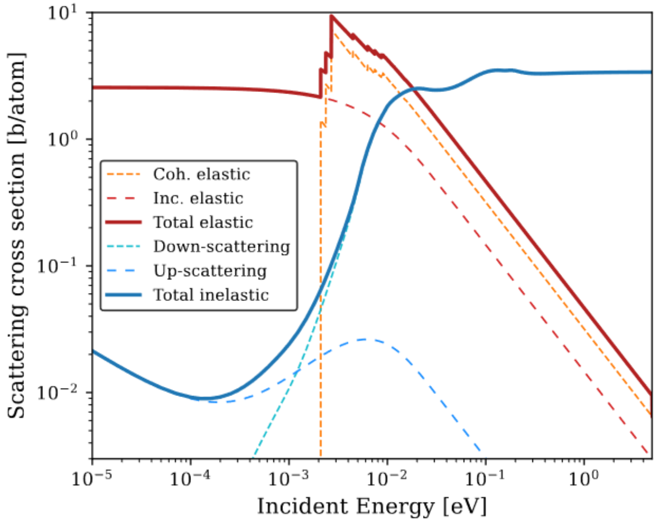
Pros

- Very low neutron absorption cross section and small nuclear mass
- Operated at 5 K
- Small upscattering cross section

Cons – long neutron path length

- Spreads out neutron cloud
- Suffer broadening of pulse by a factor of five





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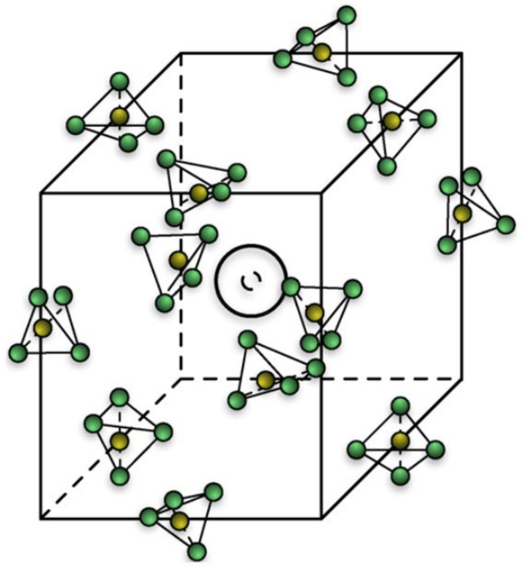

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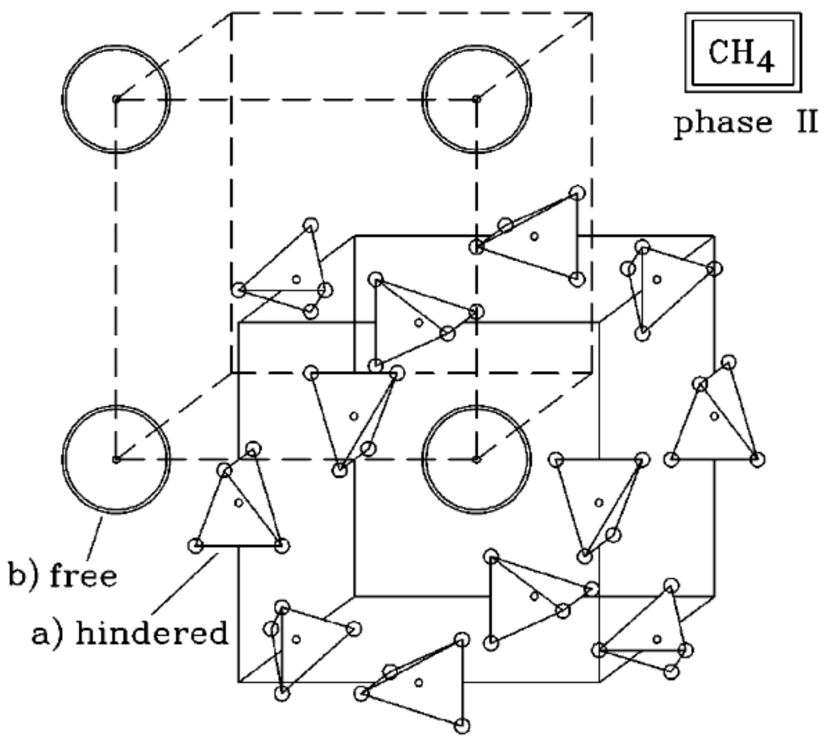
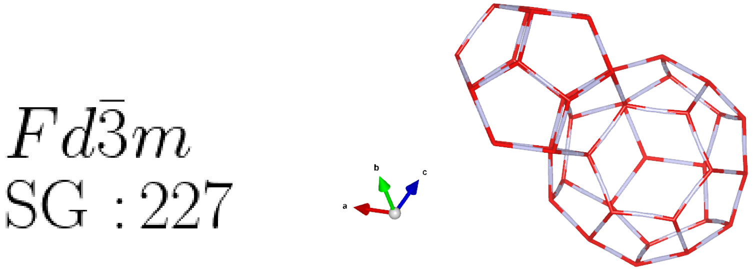


S. Grieger *et al*, J. Chem. Phys. **109** 3161–3175 (1998).

CANDIDATE VERY COLD MODERATORS

- Solid D_2
- Methane
- **Clathrates – THF-hydrates, methane hydrate**

- Inclusion compounds containing nanovoids
- Very large unit cell; a ~ 17 Å
- Cages can host guest molecules
  - ➢ THF - C_4H_8O ()
  - ➢ Oxygen - O_2 (triplet GS with zero-field splitting of 0.4 meV)
  - ➢ Methane - CH_4 (discussed previously)



A. Falenty *et al*, Nature **516** pp. 231-233 (2014).

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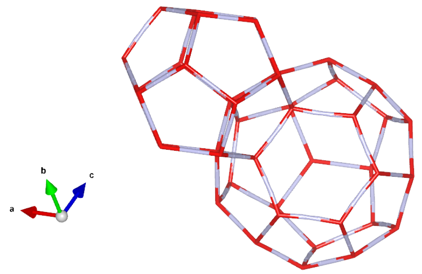
$Fd\bar{3}m$

SG : 227



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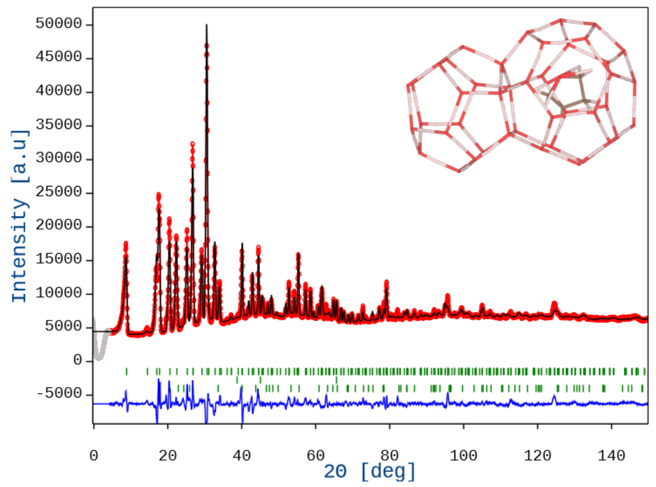

V. Czamler *et al*, EPJ Web of Conferences **286** 05004 (2023).

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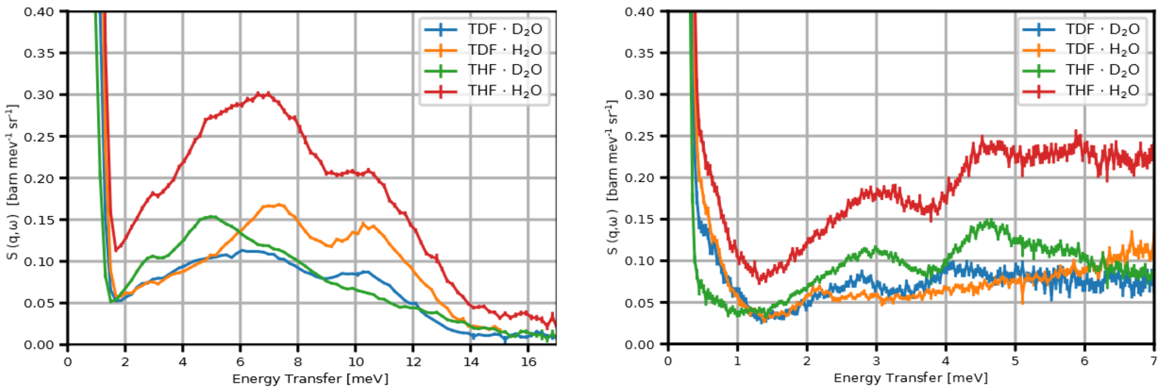
  - ➢ Methane - CH_4 (discussed previously)
- HighNESS - Cross sections developed for THF-clathrates
- Methane clathrate advantage over solid methane?
- THF-hydrate high albedo for cold neutrons



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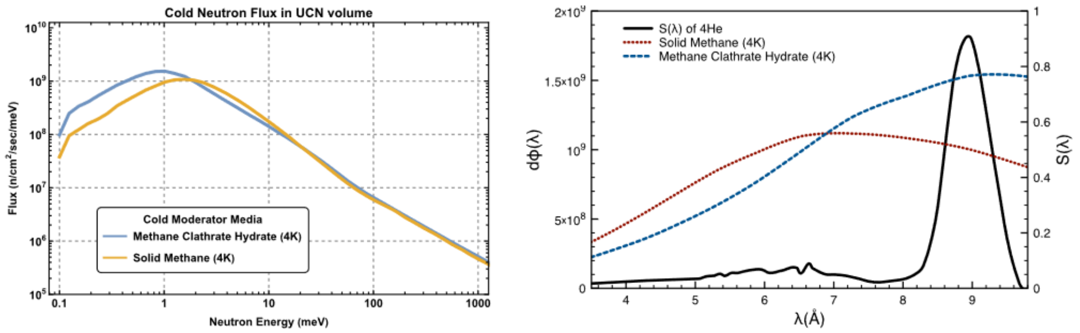

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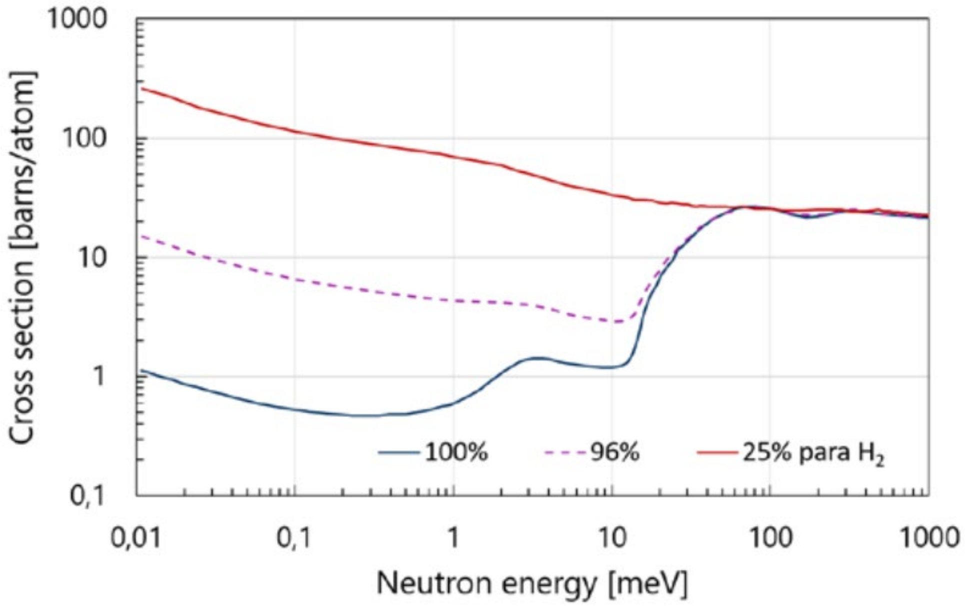
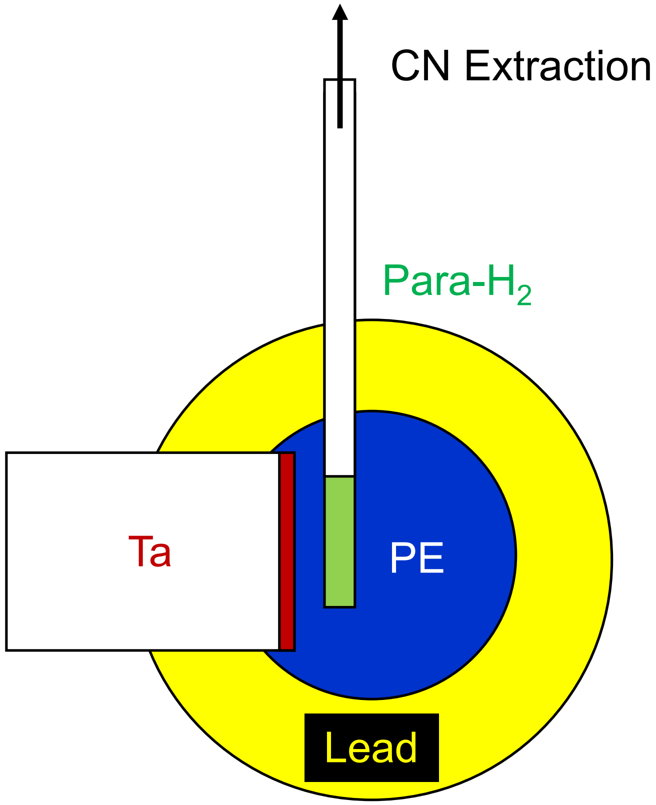
HIGH BRILLIANCE MODERATOR DESIGN

Compact 2D Cold Parahydrogen Moderator

H_2 Scattering Cross Section at 20K





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