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# Characterization of Solid Pre-Moderators for Coupled Cold Neutron Sources

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# Introduction

# Why solid pre-moderators?

## Current baseline

Pre-moderators thermalize fast & epithermal neutrons before the cryogenic cold volume. SNS coupled H<sub>2</sub> moderator uses a **water pre-moderator** – scattering kernel **fixed** at operating conditions.

## Solid alternative

A **solid, hydrogen-rich** pre-moderator offers new design flexibility:

- TSL governed by **phonon spectrum** & **VDOS**
- Changing  $T$  alters  $\frac{d^2\sigma}{d\Omega dE'} directly$
- At suitable  $T$ , can **reflect cold neutrons** back into moderator

*This work investigates several solid hydrides as candidates.*

## Key insight

**Temperature** → **new operational degree of freedom**

Spectral tuning *without* modifying the hydrogen moderator itself.

Water pre-mod  
(**fixed** TSL)

→ Single spectrum

Solid pre-mod  
(**tunable** TSL)

→ **Variable** spectrum

# Study scope: materials × temperatures × thicknesses

## Candidate materials

Material	$\rho$ (g cm <sup>-3</sup> )	$n_{\text{H}}$ (10 <sup>22</sup> cm <sup>-3</sup> )
<b>YH<sub>2</sub></b>	4.30	5.7
<b><sup>7</sup>LiH</b>	0.80	6.1
MgH <sub>2</sub>	1.45	6.6
<b><sup>15</sup>NH<sub>3</sub></b>	0.70	7.0
<b>ZrH<sub>2</sub></b>	5.61	7.2
<b>BeH<sub>2</sub></b>	0.76	8.3
H <sub>2</sub> O (ref.)	1.00	6.7

## Performance metrics

- **Time-integrated brightness** at representative viewing positions
- **FWHM pulse width** – TOF instrument performance

$$n_{\text{H}} = \rho N_{\text{A}} n_{\text{H}}^{\text{mol}} / M$$

where  $\rho$  = density,  $M$  = molar mass,  $n_{\text{H}}^{\text{mol}}$  = H per formula unit.

**Temperature scan:** 100 K → 200 K → 293.6 K → 400 K | multiple pre-moderator **thicknesses**

# Monte Carlo Model

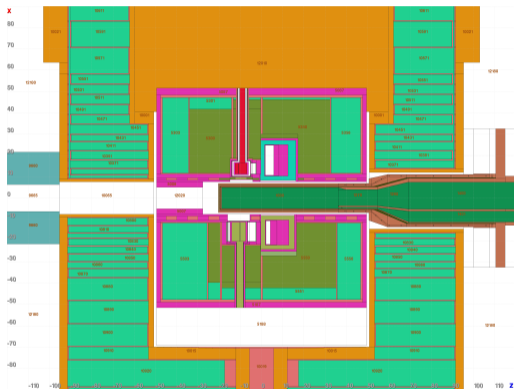
# MCNP6 model of the SNS target–moderator–reflector assembly

## Model components

- Proton target region (Hg)
- All 4 SNS moderator types (coupled/decoupled)
- Coupled **Be reflector**
- **Inner Reflector Plug (IRP)** with key as-built geometry features
- Representative instrument **viewing geometry**
- Fixed  $10 \times 12 \text{ cm}^2$  moderator viewport

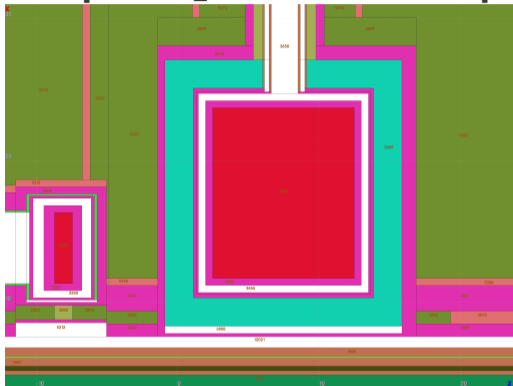
## Source & data

1.3 GeV charged proton beam,  $7 \times 20 \text{ cm}^2$  footprint  
 $10^6$  histories/case, ENDF/B-VIII.1 + custom TSL

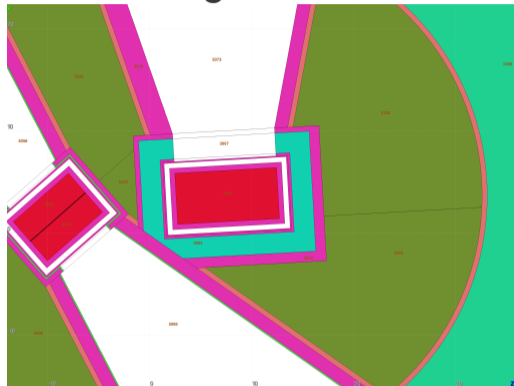


**X-Z cross-section of the SNS target–moderator assembly.** Cell numbers annotated.

## Coupled H<sub>2</sub> moderator and pre-moderator region



**X-Z midplane.** H<sub>2</sub> moderator (red), pre-moderator cavity (cyan), Al vessel walls (purple), Be reflector (olive).



**Y-Z upper plane.** Moderator, pre-moderator, beamline extraction guides, and cylindrical Be reflector.

# Parametric study: tally and simulation matrix

## Brightness tally (F55:n)

Point detector at **BL5** – downstream of coupled H<sub>2</sub> moderator with pre-moderator

- Equal-lethargy energy bins:  $10^{-11}$ – $10^6$  eV
- Time bins in decades for pulse structure
- One tally definition retained for all cases

Measures energy- and time-dependent **brightness**; the same tally is post-processed to extract integrated brightness and pulse-width trends on a consistent basis.

## Simulation matrix

**6 materials** × **4 temperatures** × **multiple thicknesses**

- Baseline: H<sub>2</sub>O pre-mod at 293.6 K for direct comparison
- Pre-moderator surrounds coupled H<sub>2</sub> volume;  
nominal thickness  $\approx 2$  cm (parametrized)
- Template-driven input generation
- Temperature-dependent  $S(\alpha, \beta)$  libraries
- $\sim 50$  cases total in parametric sweep

# Thermal Scattering Data: tslforge

# tslforge: thermal scattering ACE production pipeline

## 6-phase pipeline

- 1 VDOS extraction & **preflight** validation
- 2 TSL ENDF generation via **NCrystal**
- 3 **LEAPR** thermal scattering law processing
- 4 RECONR → BROADR → **THERMR** → **ACER**
- 5 NCrystal  $\sigma(E)$  component diagnostics
- 6 Dual-route comparison plots & cross-checks

## Configuration & automation

- **JSON config-driven**: material defs,  $\alpha/\beta$  grid points, elastic options
- **External LEAPR**: import pre-built decks with runtime grid overrides
- **ENDF parsers**: MF3/MF7 via `endf-parserpy*` for extraction & validation
- **Audit trail**: resolved config, manifests (JSON/YAML), screen logs

Materials: <sup>7</sup>LiH, YH<sub>2</sub>, ZrH<sub>2</sub>, MgH<sub>2</sub>, BeH<sub>2</sub>, <sup>15</sup>NH<sub>3</sub> across 100–400 K

\* [github.com/IAEA-NDS/endf-parserpy](https://github.com/IAEA-NDS/endf-parserpy)

# TSL data: evaluated libraries, VDOS-derived kernels, and verification

## Evaluated TSL (ENDF/B-VIII.1, JEFF-4)

<sup>7</sup>LiH, YH<sub>2</sub>, ZrH<sub>2</sub>, MgH<sub>2</sub>

Mixed elastic: coherent + incoherent contributions

## New kernels from VDOS

BeH<sub>2</sub> – VDOS from ab initio lattice dynamics\*

<sup>15</sup>NH<sub>3</sub> – VDOS computed in-house;  
liquid 220 K via external LEAPR decks

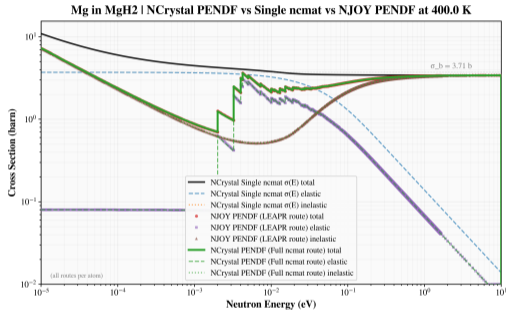
## Dual-route verification

THERMR PENDF  $\sigma(E)$  per element from **NJOY** and **NCrystal**:

- High- $E$  asymptote  $\rightarrow \sigma_{\text{free}}$
- **Mixed** coherent (Bragg) + incoherent elastic
- Scattering component decomposition (elastic, inelastic, coh., incoh.)
- $\sigma(E)$  comparison: NJOY vs NCrystal

\* M. L. Zerkle et al., *Thermal Neutron Scattering Law for Beryllium Hydride*, NPIC&HMIT 2012.

# Dual-route cross-section validation



**Mg in MgH<sub>2</sub>.** NCrystal full-material vs single-element surrogate vs evaluation through NJOY THERMR at 400 K.

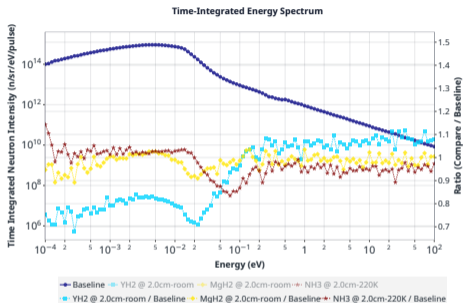
## Four production routes

- **Full-material** NCrystal route  
ncmat2endf → per-element ENDF → THERMR → ACE
- **Single-element surrogate** route  
per-element NCMAT from VDOS → ACE
- **Evaluation** through NJOY THERMR  
evaluated TSL ENDF → THERMR → ACE
- **NJOY LEAPR** vs single-element surrogates  
VDOS → LEAPR → THERMR → ACE

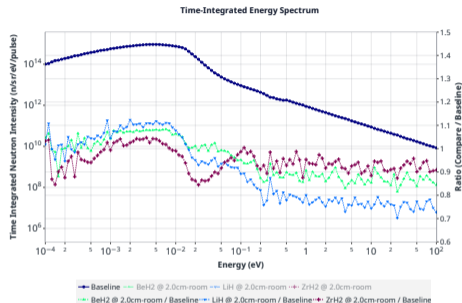
Agreement across routes validates consistency.  
Same workflow for **all materials and temperatures.**

# Results

# Results: Material Comparison



A: YH<sub>2</sub> / MgH<sub>2</sub> / <sup>15</sup>NH<sub>3</sub>

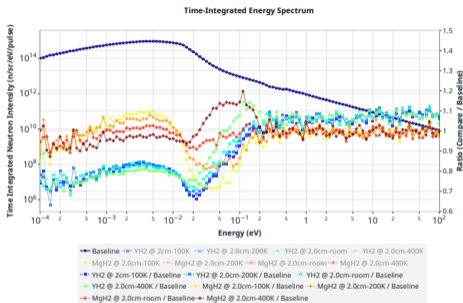


B: BeH<sub>2</sub> / <sup>7</sup>LiH / ZrH<sub>2</sub>

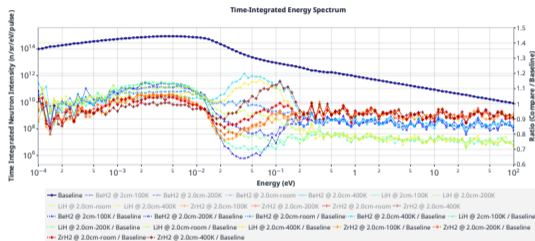
## Pre-moderator screening at 2.0 cm, room temperature

- Replacing the water pre-moderator with BeH<sub>2</sub> yields the broadest gain across the cold (1 meV to 10 meV) and thermal (10 meV to 100 meV) windows that feed the coupled H<sub>2</sub> moderator; <sup>7</sup>LiH enhances selectively near the cold peak but falls off at thermal energies.
- Among Group A hydrides, MgH<sub>2</sub> tracks closest to baseline at epithermal energies, driven by its water-like  $n_H$  and low Mg absorption; YH<sub>2</sub> provides no cold-region benefit. <sup>15</sup>NH<sub>3</sub> is the only liquid candidate, tested at 220 K, and shows a modest ~3% cold-region gain.
- BeH<sub>2</sub> and <sup>7</sup>LiH are advanced to the thickness and temperature scoping as the leading candidates.

# Results: Temperature Dependence



**A:** YH<sub>2</sub> and MgH<sub>2</sub>, 100 K, 200 K, 293.6 K and 400 K.

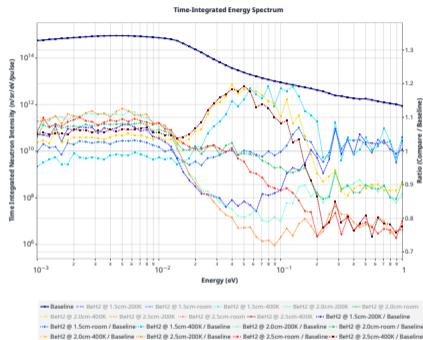


**B:** BeH<sub>2</sub>, <sup>7</sup>LiH, ZrH<sub>2</sub>, 100 K, 200 K, 293.6 K and 400 K.

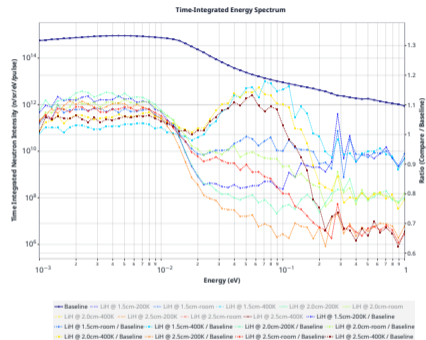
## Temperature sensitivity at 2.0 cm across all candidates (1 meV to 100 meV)

- **Group A:** MgH<sub>2</sub> cold gain < 10%; YH<sub>2</sub> high absorption (> 1 b) reduces cold spectrum by ~20%. Warming raises the epithermal ratio.
- **Group B:** BeH<sub>2</sub> and <sup>7</sup>LiH reach ~14% cold gain at 100 K; warmer operation shifts benefit toward the thermal window.
- <sup>7</sup>LiH most suppressed at epithermal energies regardless of temperature; ZrH<sub>2</sub> moderate gain.

# Results: Thickness Scoping



**BeH<sub>2</sub>**: 1.5 cm, 2.0 cm and 2.5 cm × 200 K, 293.6 K and 400 K

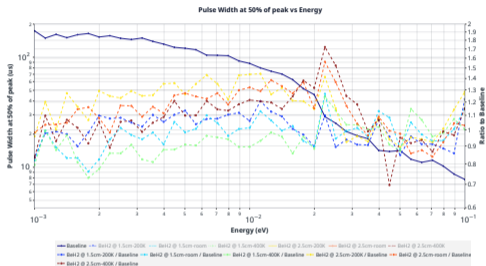


**<sup>7</sup>LiH**: 1.5 cm, 2.0 cm and 2.5 cm × 200 K, 293.6 K and 400 K

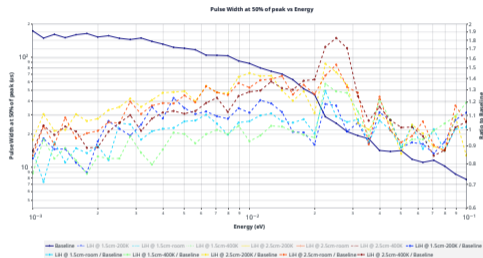
## Thickness-temperature trade-off (blues=1.5 cm, greens=2.0 cm, reds=2.5 cm)

- **BeH<sub>2</sub>**: At 2.5 cm/400 K: ~5% cold gain, ~20% thermal gain – favorable for the coupled moderator even at higher temperatures and thicknesses.
- **<sup>7</sup>LiH**: Up to ~15% cold gain at 2 cm/low-*T*; at 2.5 cm and low-*T* thermal ratio drops to ~0.6 (~40% loss).
- **Implication**: BeH<sub>2</sub> offers a tunable design space; <sup>7</sup>LiH is geometry-constrained but effective at thin layers.

# Results: Pulse Shape and FWHM



BeH<sub>2</sub> – FWHM vs energy



<sup>7</sup>LiH – FWHM vs energy

## Pulse-width impact (blues=1.5 cm, reds=2.5 cm)

- **BeH<sub>2</sub>**: FWHM ratio  $\approx 1.0$  at 1.5 cm; rises to  $\sim 1.2$ – $1.4$  at 2.5 cm in the thermal window – scales with moderation path length.
- **<sup>7</sup>LiH**:  $\sim 1.0$ – $1.1$  at 1.5 cm;  $\sim 1.3$ – $1.5$  at 2.5 cm. Higher temperature increases broadening. LiH broadens more than BeH<sub>2</sub> at equal thickness.
- **Implication**: Pulse quality preserved at 1.5 cm; 20–50% broadening at 2.5 cm. Could be acceptable for coupled moderators where resolution requirement is relaxed.

# Summary

# Solid pre-moderators: a viable pathway for cold-source gains?

## Study summary

- Five solid hydrides +  $\text{NH}_3$  benchmarked against SNS water pre-moderator (coupled-moderator MCNP6 model)
- TSL from ENDF/B-VIII.1; new kernels via NCrystal & NJOY/LEAPR for  $\text{BeH}_2$  and  $\text{NH}_3$
- $\text{BeH}_2$ : **broadest gain (~5–20% cold/thermal)**, scales favorably with thickness and temperature.
- ${}^7\text{LiH}$ : **up to ~15% cold gain** at 2.0 cm/low- $T$ ; thicker layers suppress overall spectrum
- Other candidates show minimal benefits.
- Temperature as new design DoF: warmer  $\rightarrow$  **gain shifts toward thermal window**
- Pulse broadening **10–70%** depending on temperature and thickness – tunable trade-off for coupled moderators.

## Practical challenges

- **Wigner energy:** lattice energy accumulates under irradiation  
 $\rightarrow$  **periodic replacement via cartridge-style insert**
- **Heat removal:** nuclear heating in a solid insert  
 $\rightarrow$  **dedicated cooling loop with engineered thermal contact**
- **Material integrity:** swelling, radiolysis, H redistribution  
 $\rightarrow$  **design for replaceability; validate with irradiation testing/PIE**
- **Chemical reactivity:** hydrides react with moisture  
 $\rightarrow$  **inert-atmosphere handling and hermetic encapsulation**

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