Evaluation of the Thermal Neutron Scattering Cross Sections of CaH_2

B. K. Laramee, A. I. Hawari

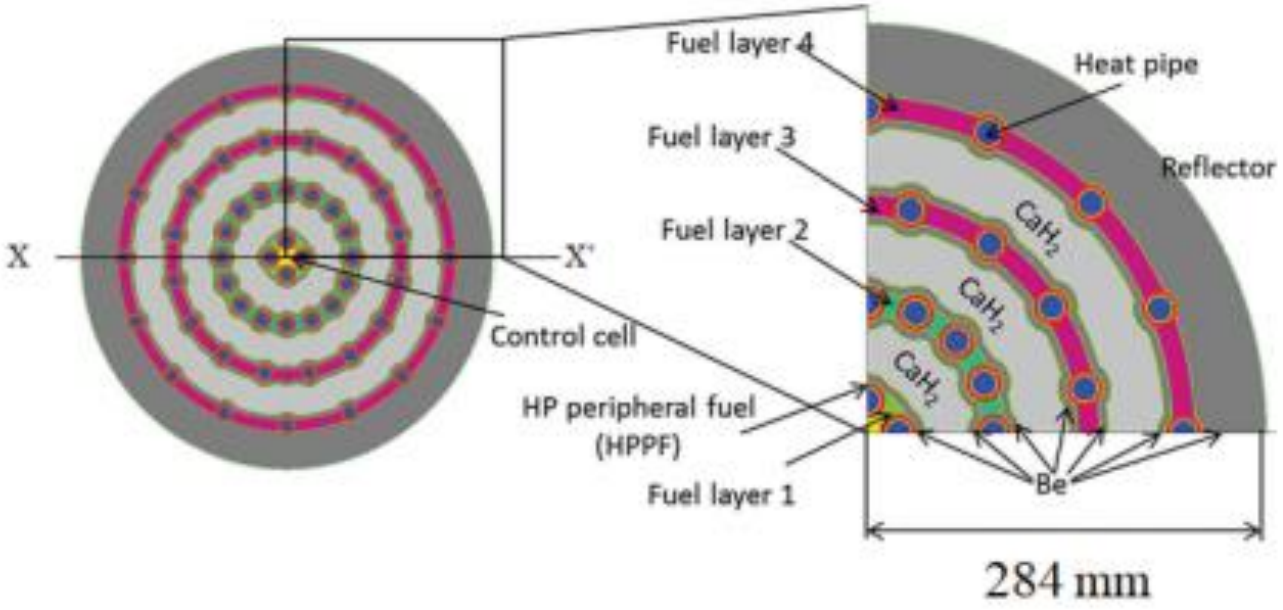
LEIP Laboratories
Department of Nuclear Engineering
North Carolina State University
Raleigh, North Carolina, USA

CSEWG, November 17, 2021 Zoom meeting
Raleigh, North Carolina, USA

Introduction

- Metal hydrides have long been considered and used as moderator materials
  - High hydrogen content
  - Good thermal stability
  - Relatively low neutron absorption
- ZrH_2 TRIGA Reactors
- Kimura & Wada (2016-2019)
  - CaH_2-moderated microreactor (<10MW)

R. KIMURA and S. WADA, "Temperature Reactivity Control of Calcium Hydride–Moderated Small Reactor Core with Poison Nuclides," *Nuclear Science and Engineering*, **193**, *9*, 1013 (2019).



Existing CaH_2 Data

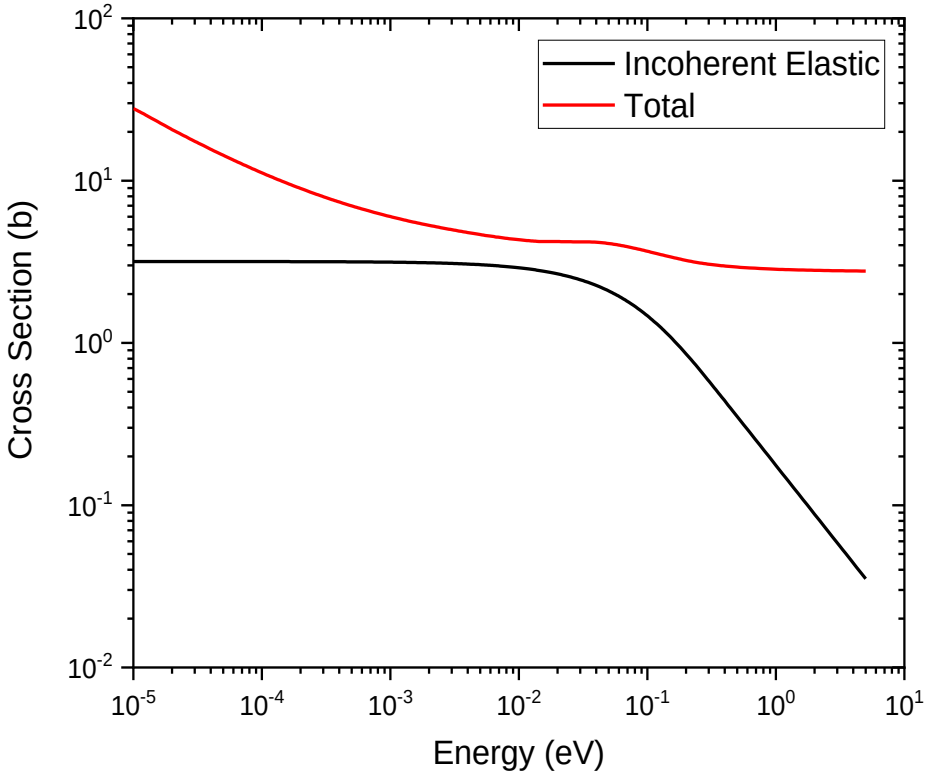
- Very little experimental data overall, including :
  - Cross Sections
  - Phonon DOS (vDOS)
  - Crystal, Material Properties
- Existing Cross Section Data :
  - No ENDF Evaluation to date
  - JEFF3.1 (O. Serot, 2005) -> JEFF3.3
    - Contains significant physical approximations

W. M MUELLER et al., Metal *Hydrides*. New York: Academic Press, Inc. (1968).

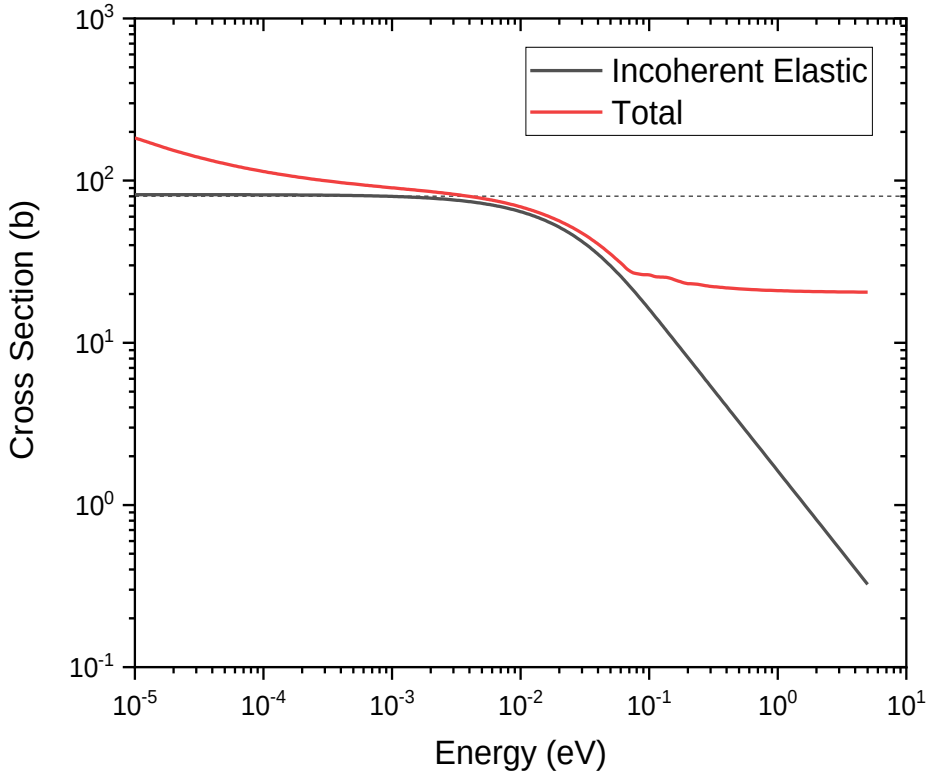
Comparison to other common moderators

Material	Slowing-Down Power [cm^{-1}]	Σ_a [cm^{-1}, 2200 m/s]	MR
H_2O	1.35	0.0222	60.9
D_2O	0.173	3.71e-5	4.68e3
$ZrH_{1.94}$	1.54	0.0065	51
CaH_2	0.974	0.0268	36.6

JEFF3.3 Data



Ca in CaH_2 Cross Sections



H in CaH_2 Cross Sections

Isotope	σ_b^{coh} [b]	σ_b^{inc} [b]
Ca (natural)	2.78	0.05
^{1}H	1.7583	80.26

Data obtained from the NIST database

O.SEROT, "New results on CaH_2 thermal neutron scattering cross sections," *AIP Conference Proceedings,* **769**, 1, 1446 (2005).

Evaluation Process

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{[\sigma_{coh} + \sigma_{inc}]}{4\pi k_B T}\sqrt{\frac{E'}{E}}S_s(\alpha,\beta)$$

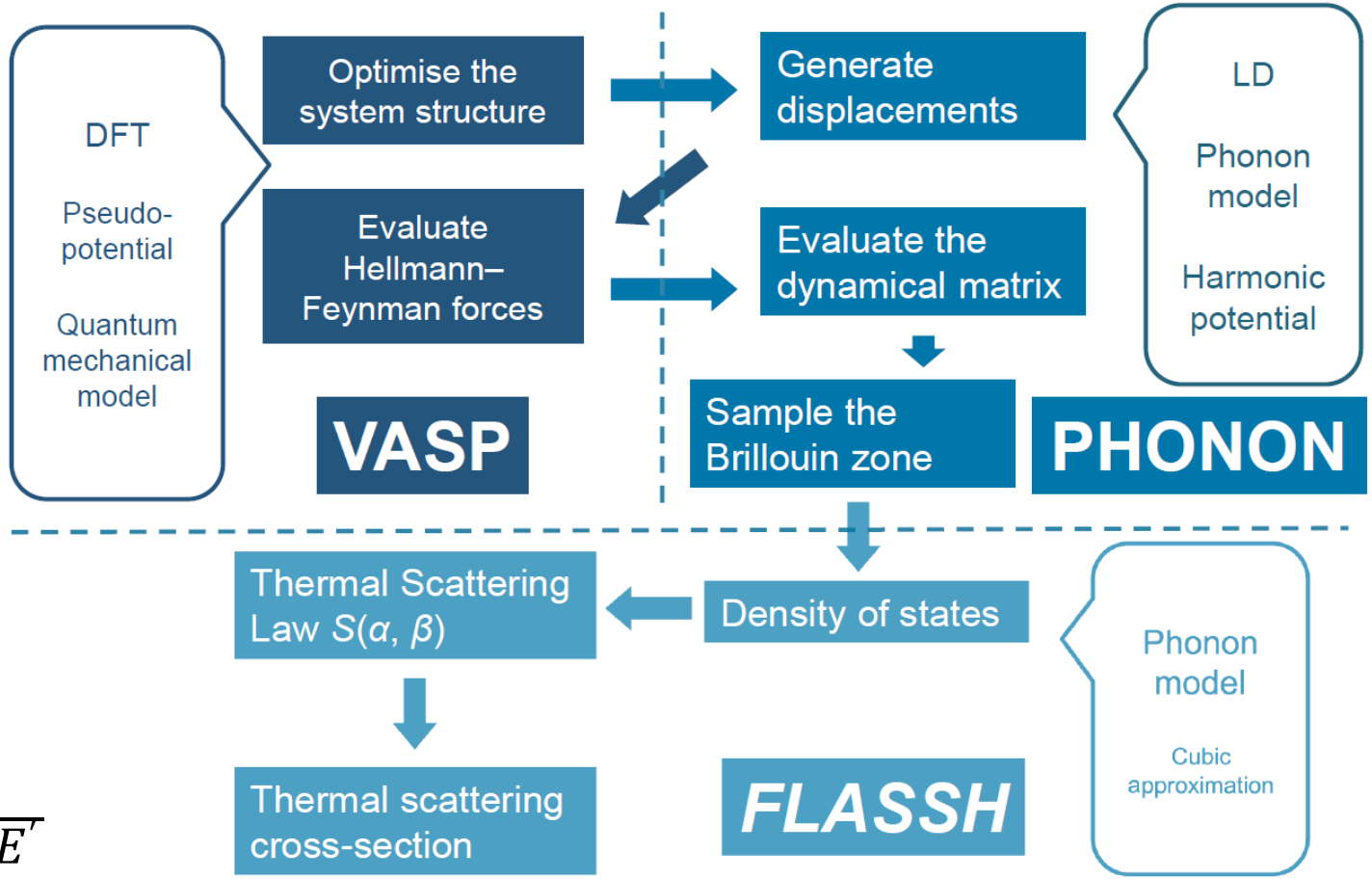
$$S(\alpha,\beta) = S_s(\alpha,\beta) + S_d(\alpha,\beta)$$

- Approximations:
  - Incoherent

    $$S_d(\alpha,\beta) = 0$$

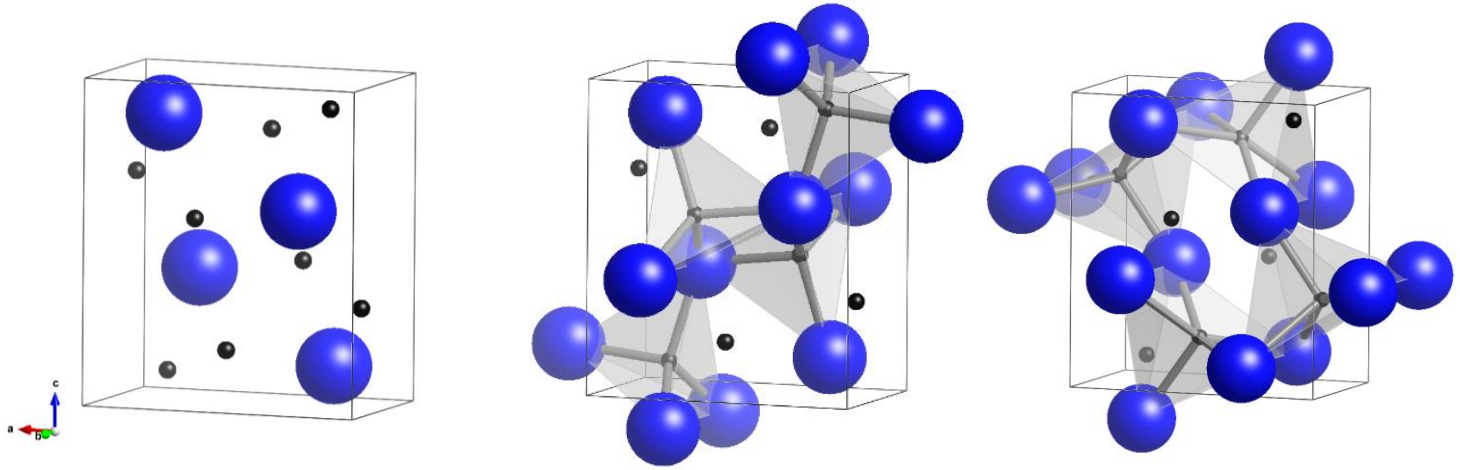
  - Gaussian
    - Harmonic

$$\beta = \frac{E' - E}{k_B T} \qquad \alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{Ak_B T}$$



CaH_2 Crystal Structure

- Orthorhombic (*Pnma*)
- 3 non-equivalent atom sites: Ca, H_1, H_2
- VASP DFT Model:
  - GGA-PBE, 675ev PW Cutoff, 9x9x9 Monkhorst-Pack k-point mesh



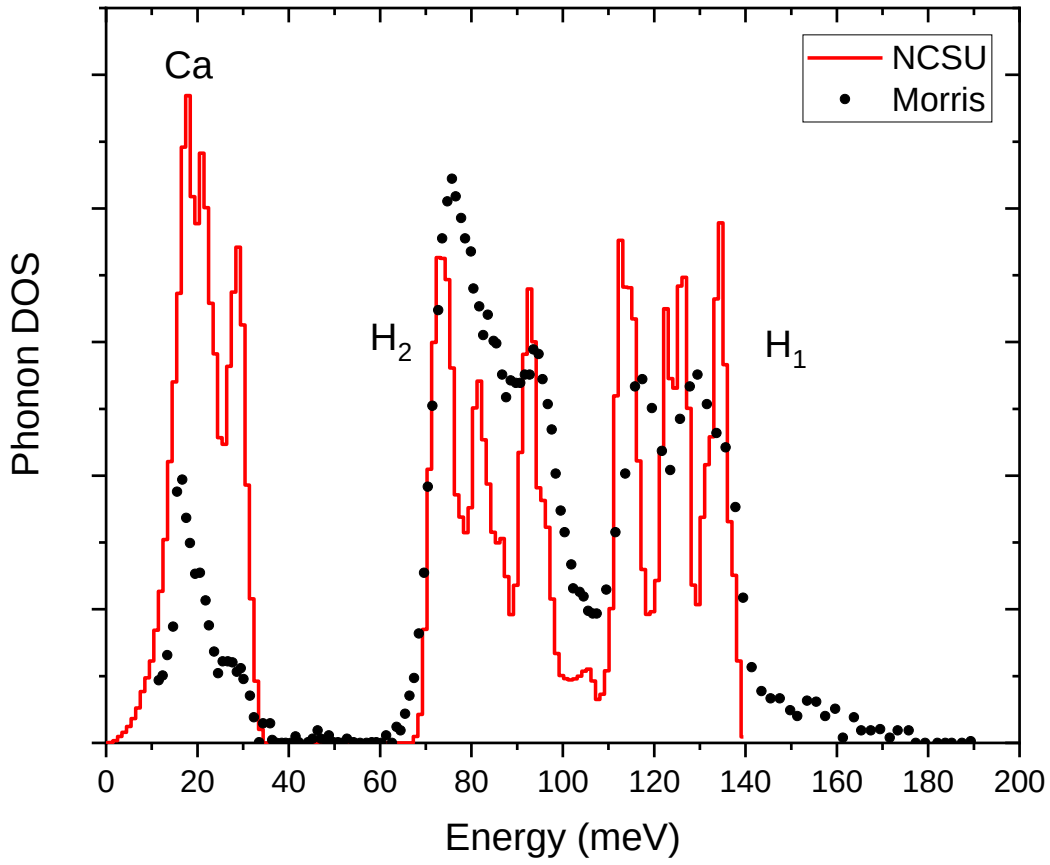
Lattice Constant	This Work	Experiment	Error (%)
a [Å]	5.92176	5.92852	0.114
b [Å]	3.57607	3.57774	0.0468
c [Å]	6.78272	6.78956	0.1007

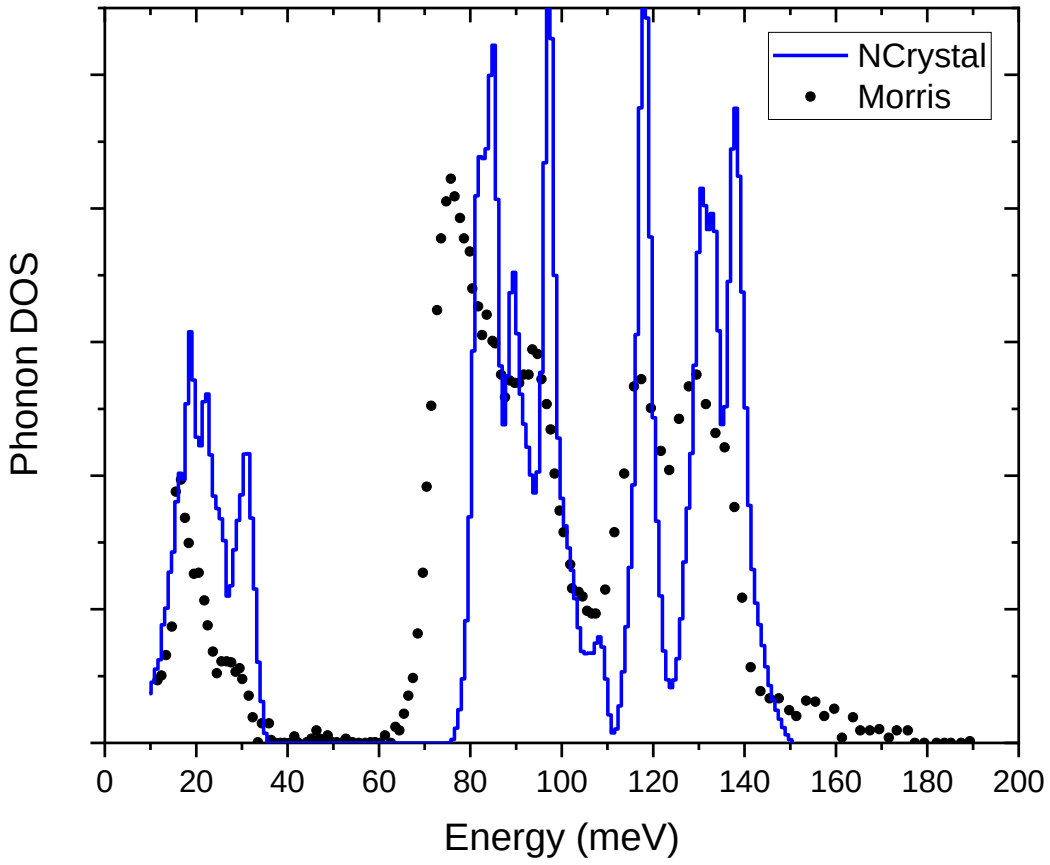
H. Wu et al., "Structure and vibrational spectra of calcium hydride and deuteride," *Journal of Alloys and Compounds*, **436**, 1-2, 51(2007)

Phonon DOS

- PHONON : 3x3x3 Supercell (324 atoms)

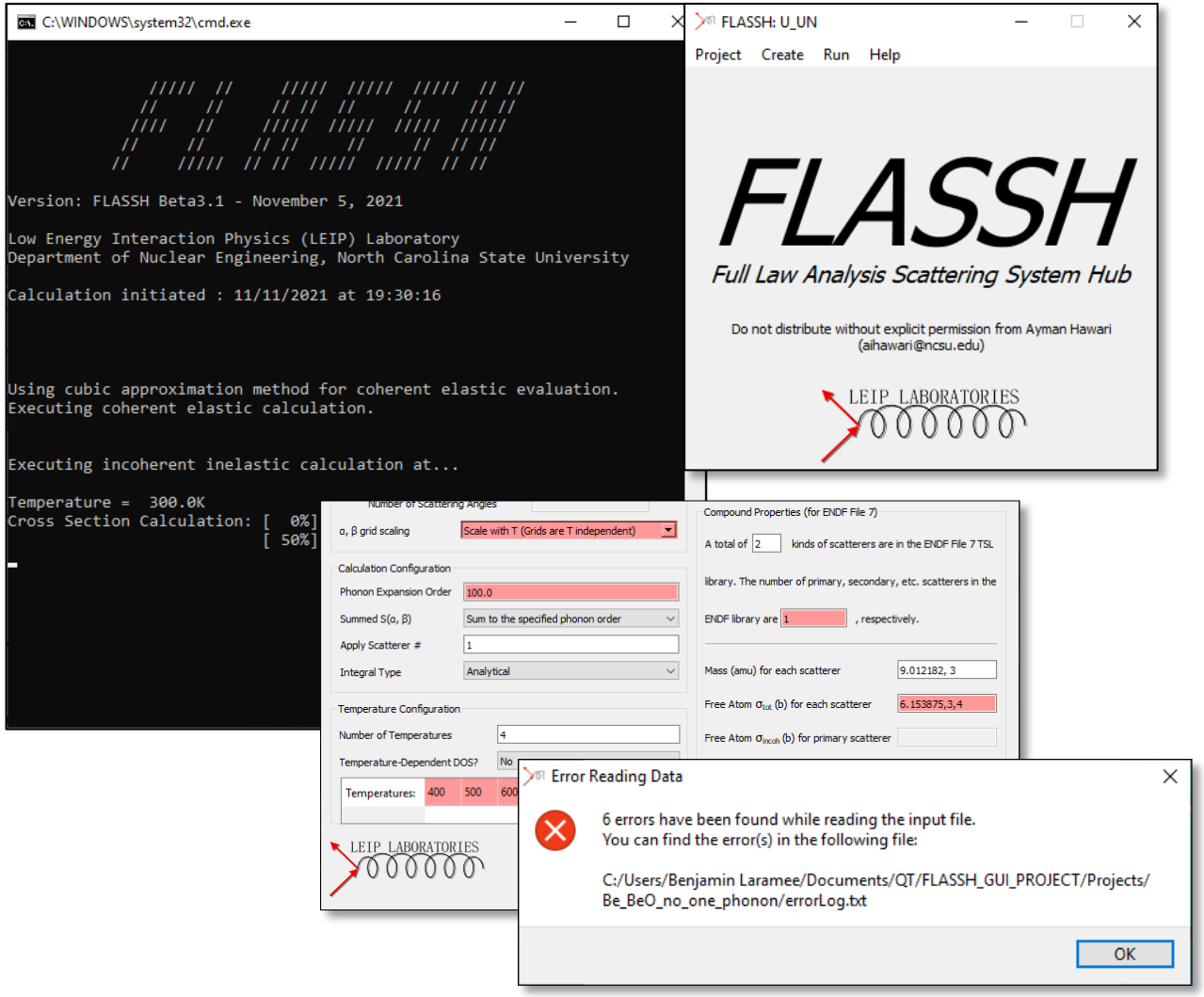
P. MORRIS et al., "Inelastic neutron scattering study of the vibration frequencies of hydrogen in calcium dihydride," *Journal of Alloys and Compounds*, **363**, *1-2*, 88 (2004).





FLASSH: Full Analysis Scattering System Hub

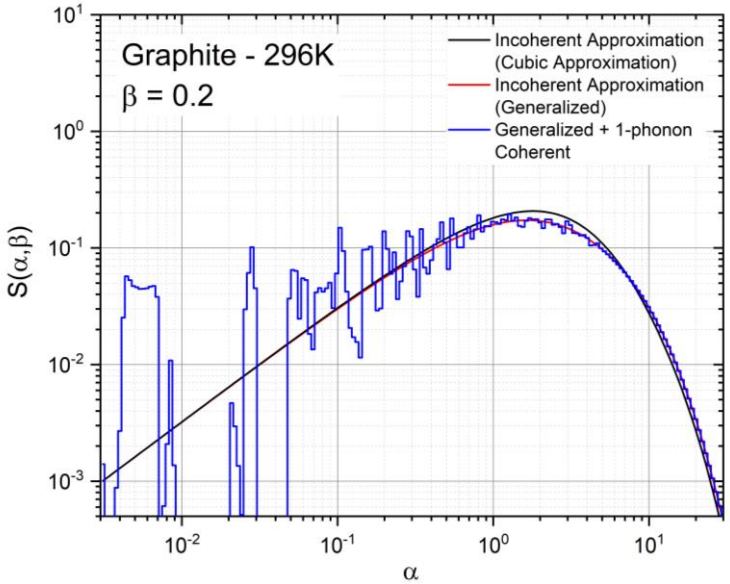
- **Motivation** - provide cross section data to support advanced reactor modeling and criticality safety
  - **High Fidelity** – TSL calculations with modern coding techniques using advanced physics
  - **Advanced Physics** – distinct (1-phonon) contributions and non-cubic formulations
  - **Graphical User Interface** – makes complex physics accessible to all users
  - **Convenient Output Formatting** – user output files, ACE files, plotted data, etc.

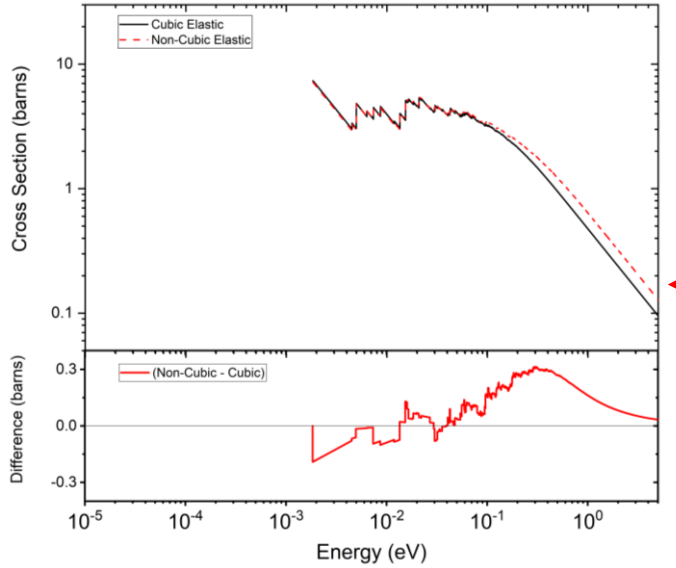


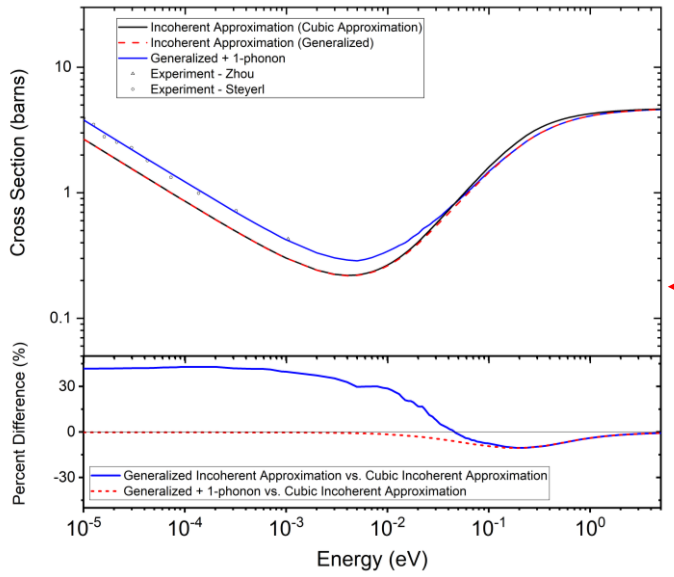
Example Error Checks

FLASSH: Full Analysis Scattering System Hub

- Advanced TSL capabilities :
  - automatic α, β gridding
  - read existing TSL to calculate cross sections
  - Loosening of the incoherent approximation: $S = S_s + S_d^1$
  - Doppler broadening capability
- Cross Sections :
  - Coherent elastic for any material
  - Noncubic formulation
  - Mixed elastic



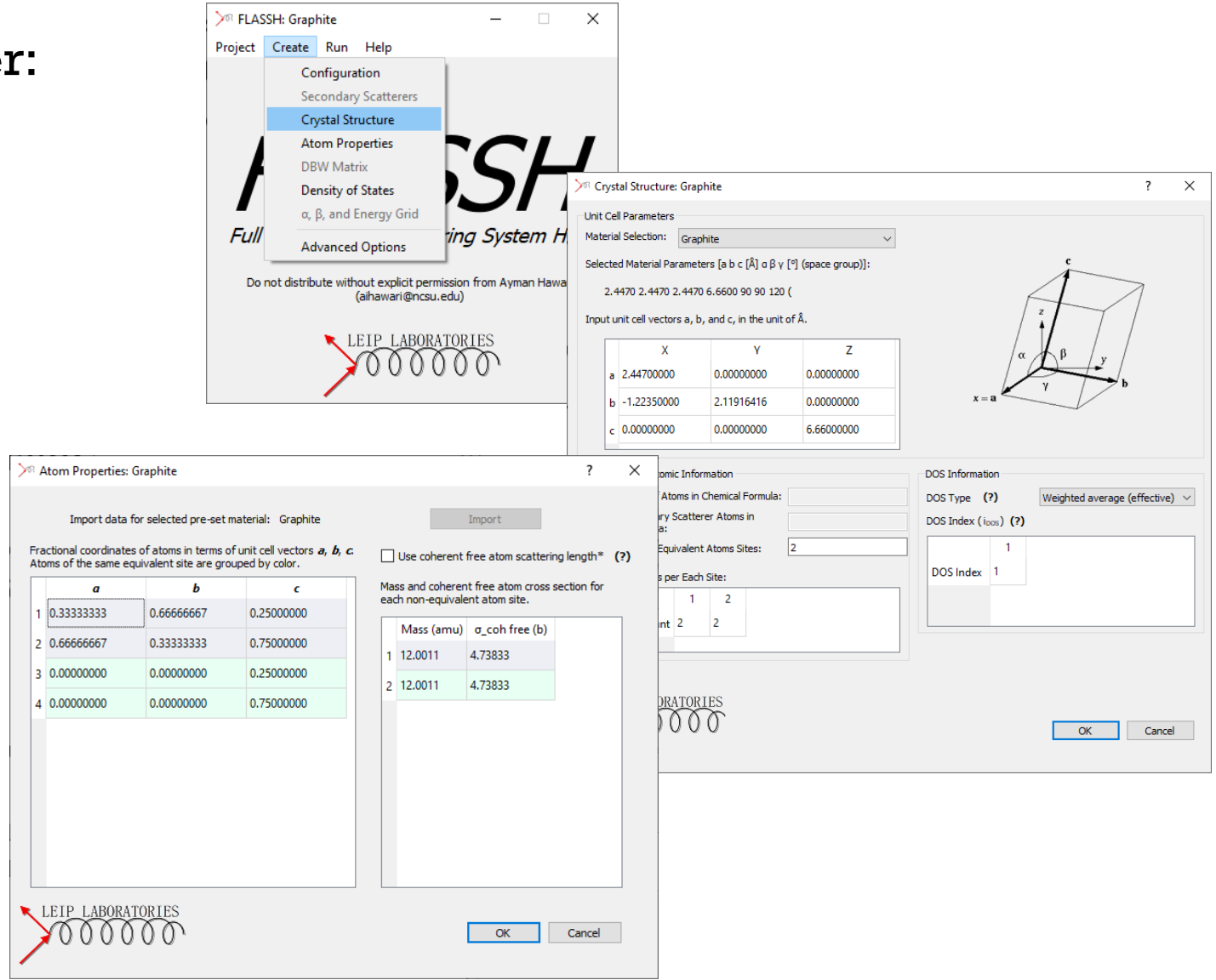




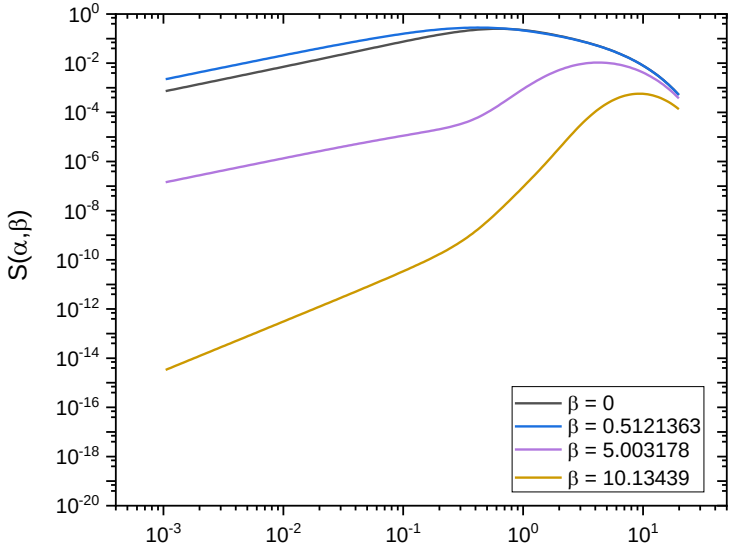
Graphite (296 K) elastic and inelastic NC and 1-phonon impacts

FLASSH: Full Analysis Scattering System Hub

- Making the evaluator's job easier:
  - GUI
    - Comprehensive error checking
  - Built-in ENDF/B-VIII.0 materials
  - Convenient formatting options
    - ENDF-6 File 7 (w/ MF=1,MT=451)
    - ACE (w/ mixed elastic)
    - NJOY-LEAPR input tape
  - Plotting
    - $[\alpha, S(\alpha,\beta)]$ for select β
    - $[\beta, S(\alpha,\beta)]$ for select α
    - Cross Sections
      - Temperature comparisons for all data
      - All contributions and total cross section
  - FUDGE/GNDS Compatibility
    - C++ GUI & Python

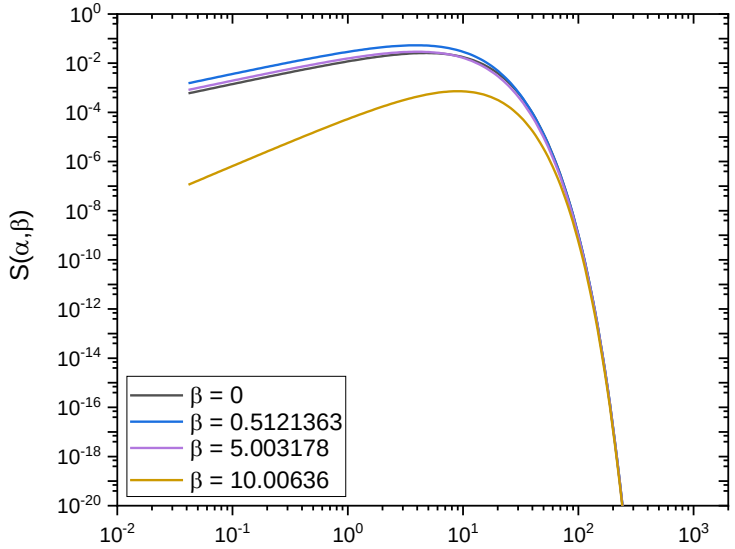


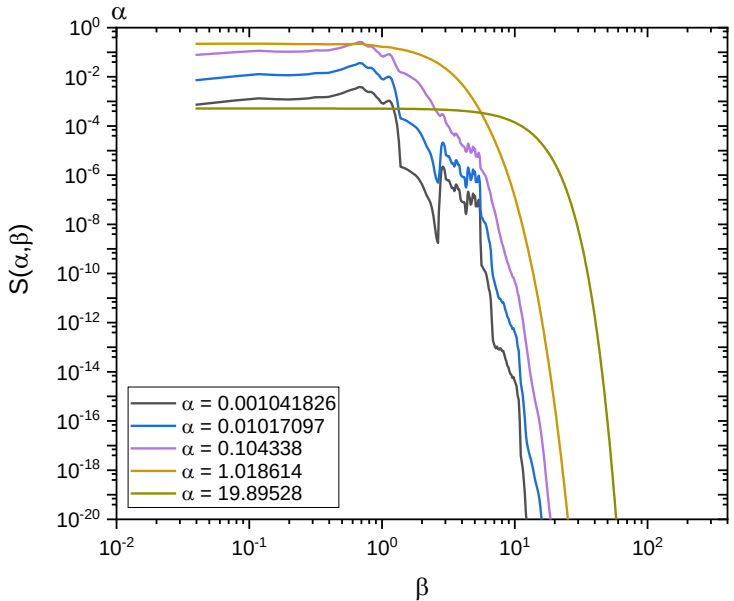
CaH_2 TSLs



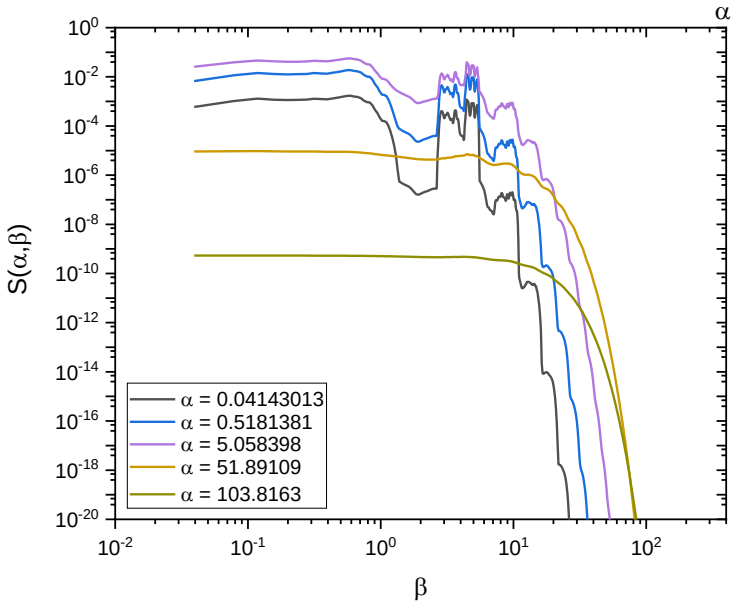
Ca : $S(\alpha,\beta)$ **v** α

H_1 : $S(\alpha,\beta)$ **v** α



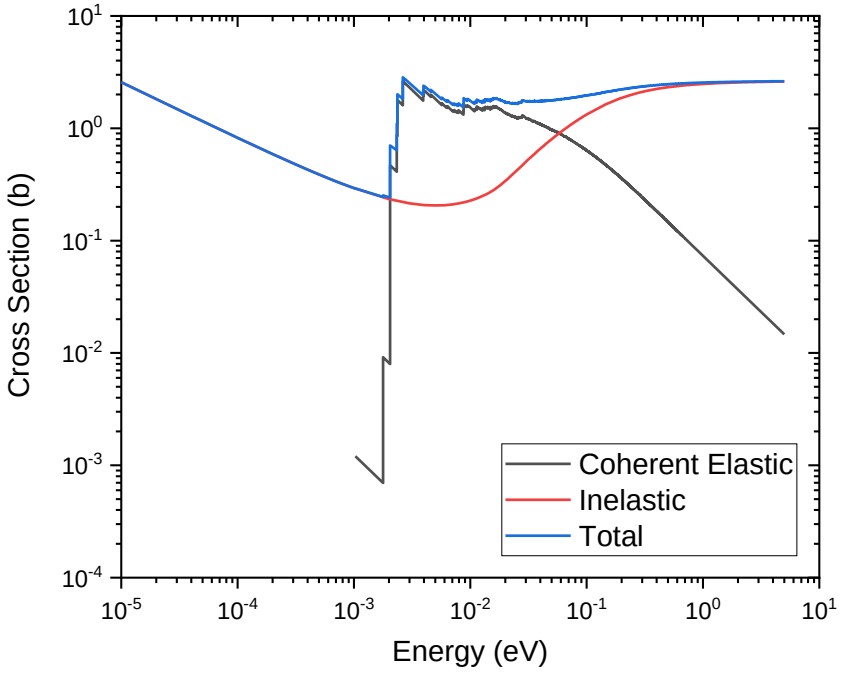


Ca : $S(\alpha,\beta)$ **v** α



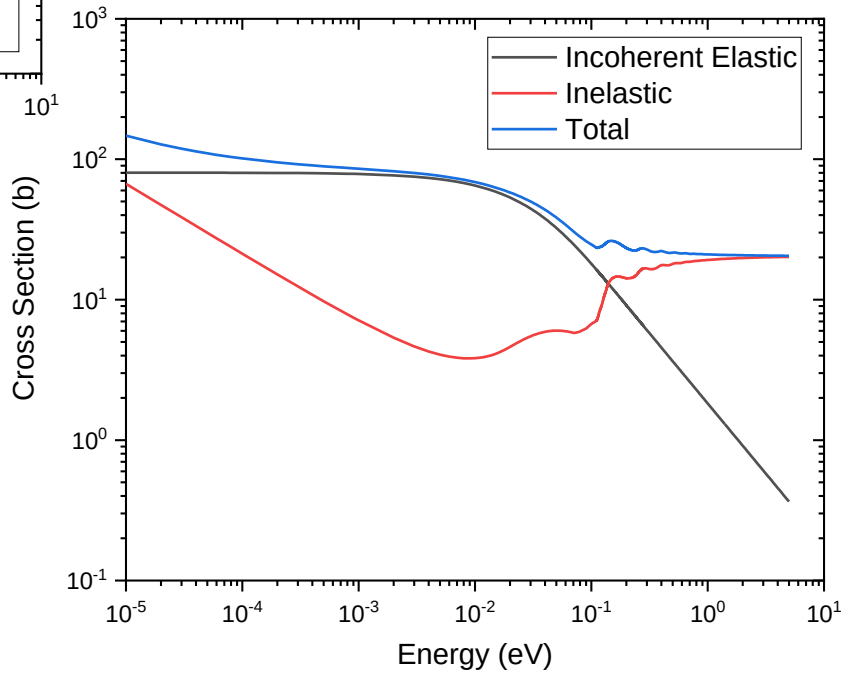
H_1 : $S(\alpha,\beta)$ **v** α

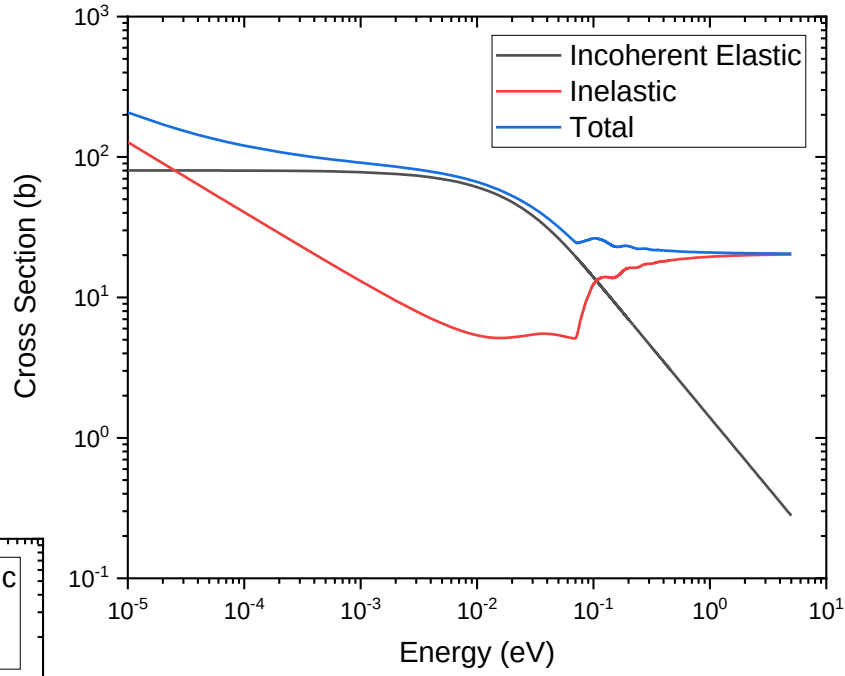
Ca in CaH_2 Cross Sections



Ca in CaH_2 Cross Sections

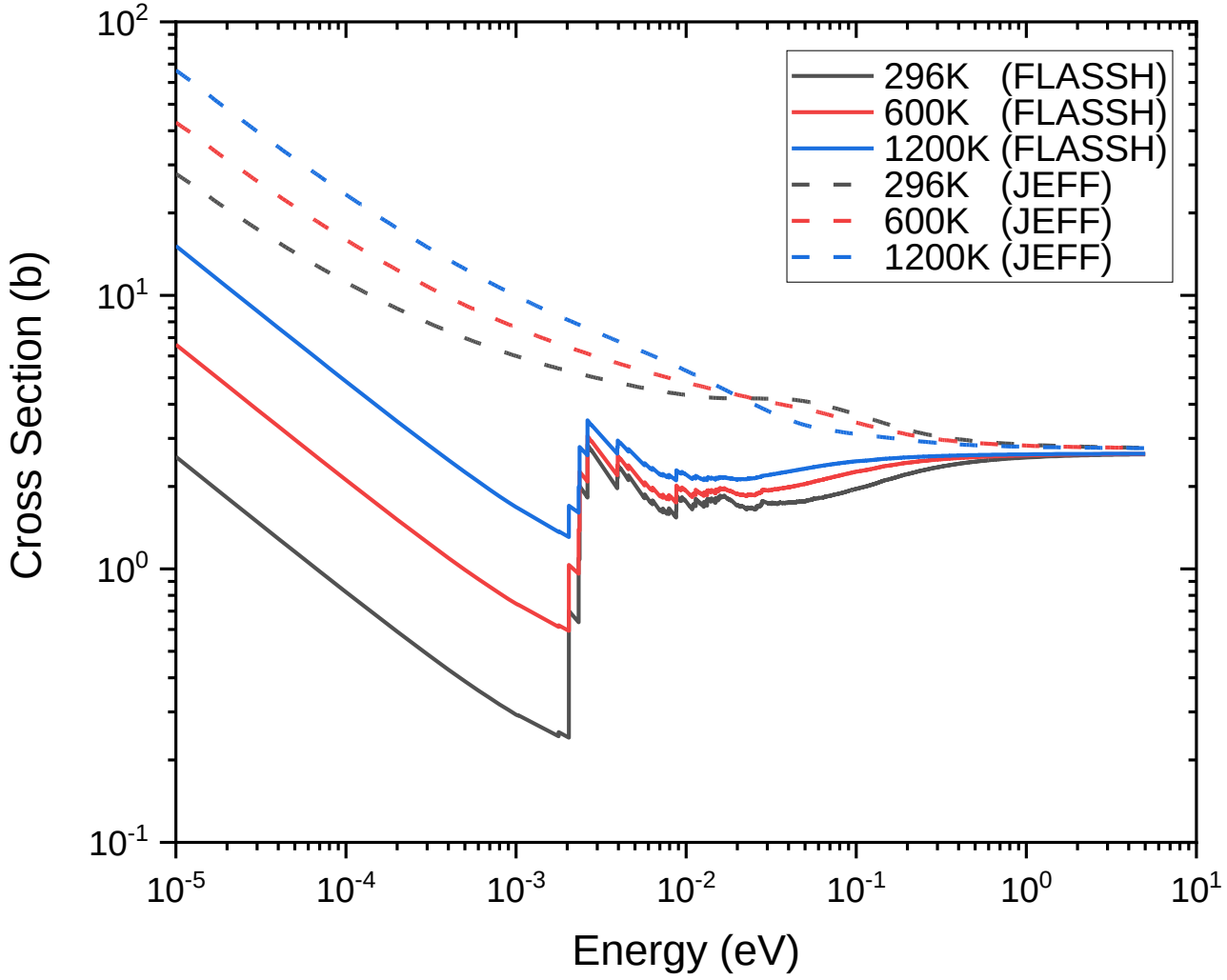
H_1 in CaH_2 Cross Sections





H_2 in CaH_2 Cross Sections

Ca in CaH_2: Comparison



CaH2 TSL for ENDF Consideration

- The following 3 evaluations have been submitted to the NNDC for consideration for ENDF/B-VIII.1 :
  - Ca in CaH_2 (MAT=59)
    - MT = 4 (Coherent)
    - MT = 2
  - H_1 in CaH_2 (MAT=8)
    - MT = 4 (Incoherent)
    - MT = 2
  - H_2 in CaH_2 (MAT=9)
    - MT = 4 (Incoherent)
    - MT = 2

```
1.590000+2 3.973374+1          -1
0.000000+0 0.000000+0           0
1.000000+0 5.000000+0           0
0.000000+0 0.000000+0           0
Ca_CaH2   LEIP LAB   EVAL-Aug21 B.K. Lara
                     DIST-
----ENDF/B-VIII.0    MATERIAL  59
-----THERMAL NEUTRON SCATTERING
------ENDF-6 FORMAT

 Temperatures = 296 400 500 600 700 800 1

HISTORY
-------
This library was produced by the Low Ener
Physics (LEIP) group at North Carolina St
Eight temperatures are available in this
scattering cross section libraries for Ca
developed using ab initio lattice dynamic
Full Law Analysis Scattering System Hub (
produce MT = 2 (coherent) and MT = 4 data
evaluation in the ENDF/B library; MAT=59
for Ca in CaH2.

THEORY
------
CaH2 has an orthorhombic crystal structur
Pnma Hermann-Mauguin space group, with th
sites. One nonequivalent site belongs to
the other two both contain hydrogen atoms
hydrogen atoms provide distinct contribut
frequency spectrum of the material and th
scattering cross sections. An evaluation
each nonequivalent hydrogen atom in CaH2,
evaluation for the metal ion. The coheren
section is stored on the calcium tape, bu
contributions from all nonequivalent site
elastic cross section of calcium is negli

REFERENCES
----------
1. A.I. Hawari, "Modern Techniques in Ine
   Scattering Analysis," Nucl. Data Sheet

2. B. K. Laramee, A. I. Hawari, " Evaluat
   Scattering Cross Sections for CaH2," T
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```
1.080000+2 9.991673-1          -1
0.000000+0 0.000000+0           0
1.000000+0 5.000000+0           0
0.000000+0 0.000000+0           0
H1_CaH2   LEIP LAB   EVAL-Feb21 B.K. Lara
                     DIST-
----ENDF/B-VIII.0    MATERIAL   8
-----THERMAL NEUTRON SCATTERING DATA
------ENDF-6 FORMAT

 Temperatures = 296 400 500 600 700 800 1

HISTORY
-------
This library was produced by the Low Ener
Physics (LEIP) group at North Carolina St
Eight temperatures are available in this
scattering cross section libraries for H1
developed using ab initio lattice dynamic
Full Law Analysis Scattering System Hub (
produce MT = 2 (incoherent) and MT = 4 da
novel evaluation in the ENDF/B library; M
chosen for H1 in CaH2.

THEORY
------
CaH2 has an orthorhombic crystal structur
Pnma Hermann-Mauguin space group, with th
sites. One nonequivalent site belongs to
the other two both contain hydrogen atoms
hydrogen atoms provide distinct contribut
frequency spectrum of the material and th
thermal scattering cross sections. As a r
evaluation has been submitted for each no
atom in CaH2.

REFERENCES
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1. A.I. Hawari, "Modern Techniques in Ine
   Scattering Analysis," Nucl. Data Sheet

2. B. K. Laramee, A. I. Hawari, "Evaluati
   Scattering Cross Sections for CaH2," T
   American Nuclear Society, 124, 2021.

3. Y. Zhu, A.I. Hawari, "Full Law Analysi
   (FLASSH)," PHYSOR 2018: Reactor Physic
   Towards More Efficient Systems, Cancun,

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                          1        4
                          7
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```
1.090000+2 9.991673-1          -1          0          0          0   9 1451
0.000000+0 0.000000+0           0          0          0          6   9 1451
1.000000+0 5.000000+0           0          0         12          8   9 1451
0.000000+0 0.000000+0           0          0         46          3   9 1451
H2_CaH2   LEIP LAB   EVAL-Feb21 B.K. Laramee, A.I. Hawari           9 1451
                     DIST-                                          9 1451
----ENDF/B-VIII.0    MATERIAL   9                                   9 1451
-----THERMAL NEUTRON SCATTERING DATA                                9 1451
------ENDF-6 FORMAT                                                 9 1451
                                                                    9 1451
 Temperatures = 296 400 500 600 700 800 1000 1200 K                 9 1451
                                                                    9 1451
HISTORY                                                             9 1451
-------                                                             9 1451
This library was produced by the Low Energy Interactions            9 1451
Physics (LEIP) group at North Carolina State University (USA).      9 1451
Eight temperatures are available in this library. The inelastic     9 1451
scattering cross section libraries for H2 in CaH2 were              9 1451
developed using ab initio lattice dynamics (AILD) [1,2]. The        9 1451
Full Law Analysis Scattering System Hub (FLASSH) was used to        9 1451
produce MT = 2 (incoherent) and MT = 4 data [3]. This is a          9 1451
novel evaluation in the ENDF/B library; MAT=9 and ZA=109 are        9 1451
chosen for H2 in CaH2.                                              9 1451
                                                                    9 1451
THEORY                                                              9 1451
------                                                              9 1451
CaH2 has an orthorhombic crystal structure belonging to the         9 1451
Pnma Hermann-Mauguin space group, with three nonequivalent atom     9 1451
sites. One nonequivalent site belongs to the metal ion, while       9 1451
the other two both contain hydrogen atoms. As a result, these       9 1451
hydrogen atoms provide distinct contributions to the overall        9 1451
frequency spectrum of the material and thus have different          9 1451
thermal scattering cross sections. As a result, a unique            9 1451
evaluation has been submitted for each nonequivalent hydrogen       9 1451
atom in CaH2.                                                       9 1451
                                                                    9 1451
REFERENCES                                                          9 1451
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1. A.I. Hawari, "Modern Techniques in Inelastic Thermal Neutron     9 1451
   Scattering Analysis," Nucl. Data Sheets 118, 172 (2014).         9 1451
                                                                    9 1451
2. B. K. Laramee, A. I. Hawari, "Evaluation of Thermal Neutron      9 1451
   Scattering Cross Sections for CaH2," Transactions of the         9 1451
   American Nuclear Society, 124, 2021.                             9 1451
                                                                    9 1451
3. Y. Zhu, A.I. Hawari, "Full Law Analysis Scattering System Hub    9 1451
   (FLASSH)," PHYSOR 2018: Reactor Physics Paving the Way           9 1451
   Towards More Efficient Systems, Cancun, Mexico, 2018.            9 1451
                                                                    9 1451
-------------------------------------------------------------------- 9 1451
                          1        451         53          0         9 1451
                          7          2          6          0         9 1451
                          7          4     151358          0         9 1451
                                                                    9 1   0
                                                                    9 0   0
1.090000+2 9.991673-1          2          0          0          0   9 7   2
8.027001+1 0.000000+0          0          0          1          8   9 7   2
         8          2                                                9 7   2
2.960000+2 1.436452+1 4.000000+2 1.633477+1 5.000000+2 1.857166+1   9 7   2
```

Summary

- CaH_2 evaluation was performed using the *FLASSH* code
  - Evaluated the coherent elastic component of Ca in CaH_2
  - Evaluated the cross sections for the nonequivalent H_1 & H_2 atom sites, as opposed to an averaged H
  - Accounted for the negative coherent scattering length of H

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Thank You!

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