ENDF status and update

33rd WPEC Meeting

13-14 May 2020 Zoom Videoconference

D. A. Brown

for the Cross Section Evaluation Working Group

National Nuclear Data Center

Brookhaven National Laboratory

BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

COVID-19 Impacts

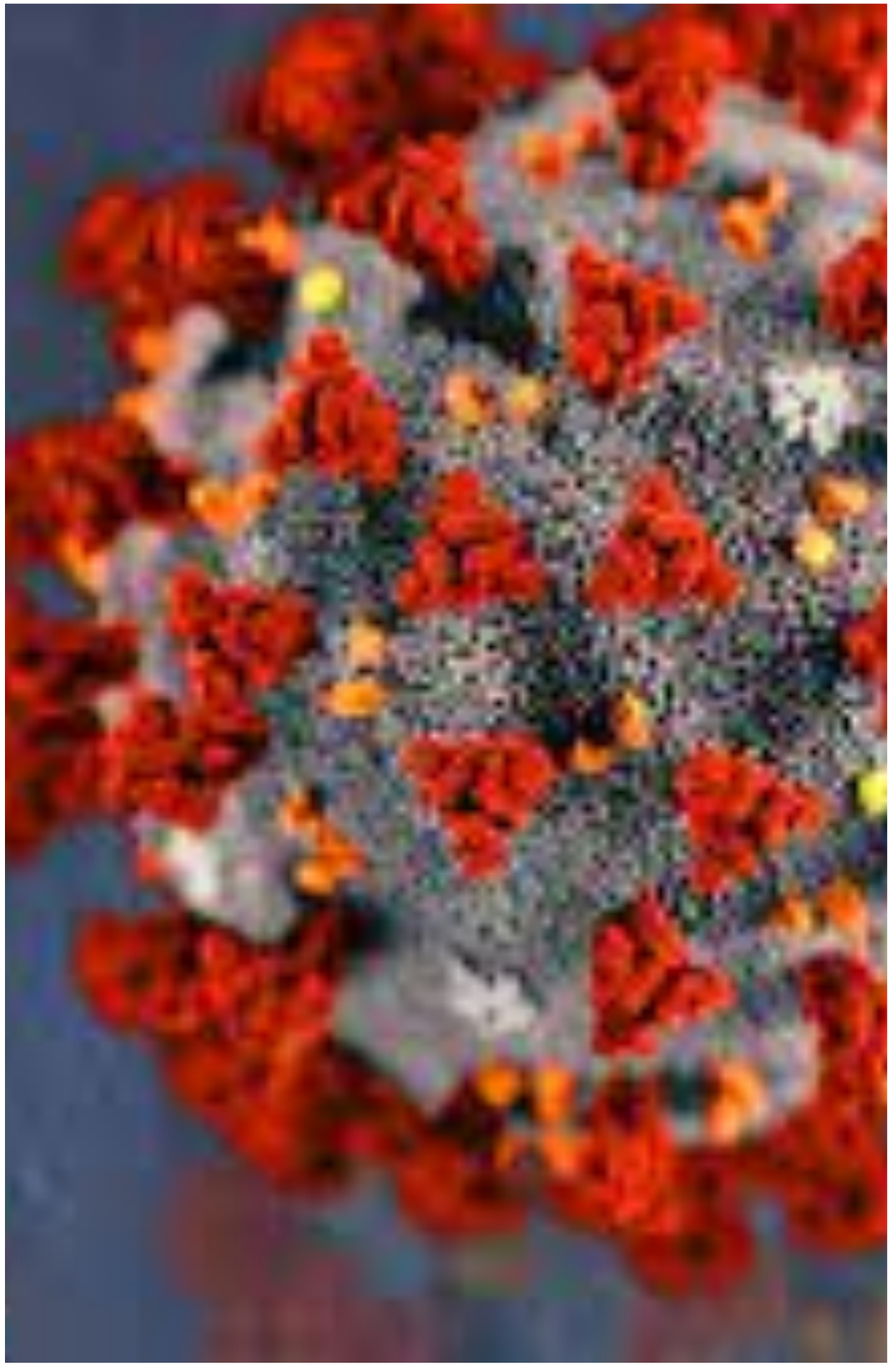
Nuclear Data Week 2020
- 100% Virtual
- 194 registered attendees
- 170 peak attendance

Cancelled 2020 mini-CSEWG & ENDF Hackathon

Mini-CSEWG 2021 to be virtual in summer

ENDF Hackathon 2021 cancelled

WANDA 2021
- 100% Virtual



2020 CSEWG Minutes are in final editing and should be ready in about a week

2020 Virtual CSEWG Meeting Minutes

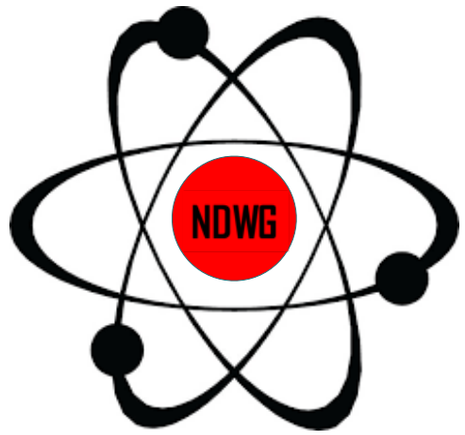
30 November-2 December 2020

Executive Committee:
Alejandro Sonzogni (BNL, chair), David Brown (BNL), Allan D. Carlson (NIST), Mark B. Chadwick (LANL, chair – Evaluation), Yaron Danon (RPI, chair – Measurements), Michael Dunn (Spectra Tech Inc., co-chair - Formats & Processing), Dorothea Wiarda (ORNL, co-chair - Formats & Processing), Densise Neudecker (LANL, chair – Covariances), Ian Thompson (LLNL), Michael Zerkle (NNL, chair – Validation)

Editor: Gustavo Nobre (BNL)

New(ish) ENDF Planning & Funding Process

The Nuclear Data Working group (NDWG)



- In FY19 we formalized the collaboration with a new charter

MISSION STATEMENT

- The goal of the Nuclear Data Working Group (NDWG) is to facilitate communication, collaboration, coordination and prioritization of nuclear data efforts across multiple program offices, the national laboratories, universities, and industry.

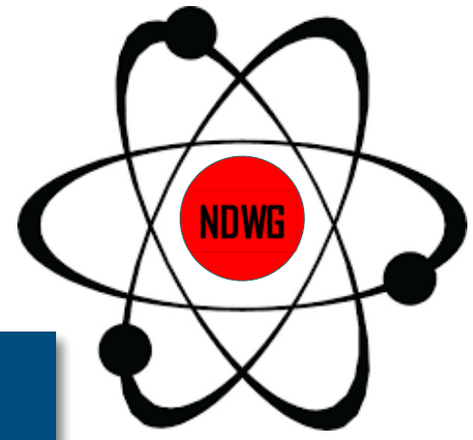
MEMBERSHIP

- Members shall be experts in their respective fields and be nominated to serve on the committee by program managers or national laboratories.
  - Up to 2 members can be nominated per program manager
  - Up to 2 members can be nominated per national laboratory

Please contact me romanoce@ornl.gov for information on participation

Slide from Cathy Romano (WANDA 2020)

The Nuclear Data Working group (NDWG)



- In FY19 we formalized the collaboration with a new charter

MISSION STA

- The goal o
  communic
  data effor
  universities

MEMBERSHIP

- Members s
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  - Up to 2 m
  - Up to 2 m

The NDWG/WANDA process is a valuable addition to CSEWG planning and brought several new user communities to CSEWG

http://www.nndc.bnl.gov/ndwg/

Please contact me romanoce@ornl.gov for information on participation

Slide from Cathy Romano (WANDA 2020)

WANDA 2021

25 Jan 3 Feb 2021 (Virtual)
Chaired by K. Kolos (LLNL) V. Sobes (UTK)

- **Plenary**
- **WANDA 2020 Session Reports**
- **Sessions:**
  - *Predictive Codes for Isotope Production*
    Chairs: S. Hogle (ORNL), E. O'Brien (LANL), A. Voyles (LBNL)
  - *Expanded Benchmarks & Validation for Nuclear Data*
    Chairs: J. Hutchinson (LANL), C. Percher (LLNL), M. Zerkle (NNL)
  - *Advanced Computing for Nuclear Data*
    Chairs: D. Brown (BNL), B. Goldblum (LBNL), B. Loer (PNNL), M. Mumpower (LANL), N. Schunck (LLNL), M. Smith (ORNL)
  - *Intro to Nuclear Data for Space Application*
    Chairs: M. Burkey (LLNL), L. Heilbronn (UTK), P. Peplowski (JHUAPL)
  - *Nuclear Data for Advanced Reactors and Security Applications*
    Chairs: M. Elsawi (PNNL), N. Thompson (LANL), W. Wieselquist (ORNL)
  - *The Human Pipeline for Nuclear Data*
    Chairs: L. Bernstein (UCB/LBNL), Y. Danon (RPI), E. McCutchan (BNL), J. Ressler (LLNL)
- **Funded Project Reports**
- **WANDA 2021 Session Reports**

FY21 NDIAWG FOA

87 LOI's submitted

58 Nuclear Physics
16 "pipeline"
31 "high impact"
11 "basic science"

29 Isotope Production & NA-22

Results expected this summer

DEPARTMENT OF ENERGY
OFFICE OF SCIENCE
NUCLEAR PHYSICS

NUCLEAR DATA INTERAGENCY WORKING GROUP (NDIAWG) RESEARCH PROGRAM

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER: DE-FOA-0002440

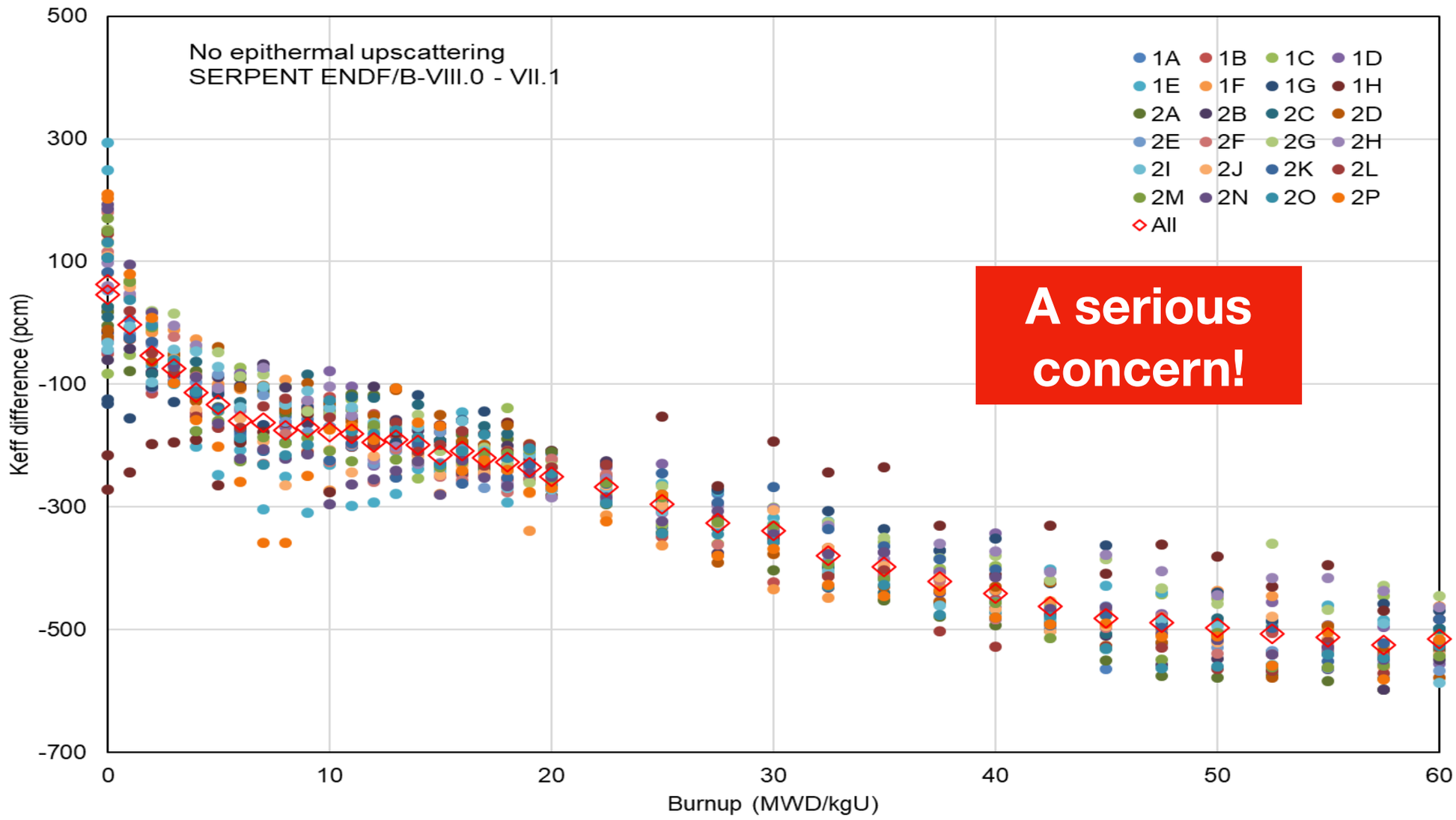
FOA TYPE: INITIAL
CFDA NUMBER: 81.049

FOA Issue Date:	**December 7, 2020**
Submission Deadline for Letters of Intent:	**January 7, 2021 at 5 PM Eastern Time (A Letter of Intent is required)**
Letter of Intent Response Date	**January 21, 2021 at 5 PM Eastern Time**
Submission Deadline for Applications:	**March 8, 2021 at 5 PM Eastern Time**

A validation concern

ENDF/B-VII.1 vs. ENDF/B-VIII.0 for Depletion

- **Reactivity underestimation**
  - VERA Depletion Benchmark Problems
    - PWR single pins and assemblies: SERPENT2 Monte Carlo
  - ENDF/B-VIII.0 reactivities are much lower
    - ^{235}U absorption cross section



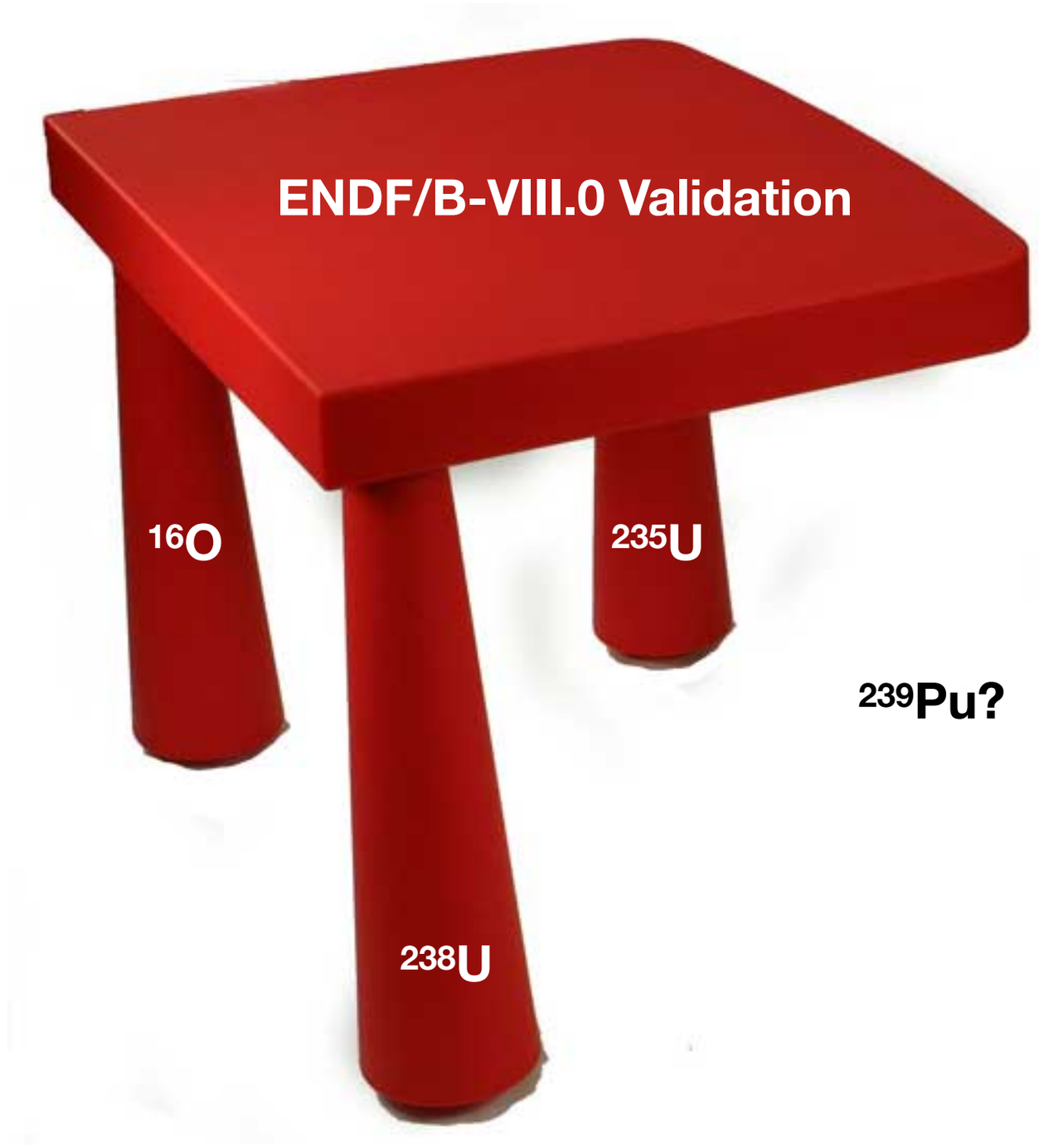
SCALE XSProc Team, CSEWG (2020)

Discussion & Conclusion

- **ENDF/B-VII.1 vs. ENDF/B-VIII.0**
  - Most influencing nuclides
    - U-238, Pu-239, O-16 and U-235
    - U-238: +300 pcm at 0 burnup & getting decreased at high burnup
    - O-16: -150 pcm at all burnup steps
    - U-235: -150 pcm at all burnup steps
    - Pu-239: -200 pcm at high burnups
  - Error cancellation
    - U-238 (positive) vs. U-235 + O-16 (negative)
  - Decay data & F.P. yield data
    - No impact
  - Thermal reactor analysis
    - Generally accepted that even ENDF/B-VII.1 underestimates keff at high burnup
    - No epithermal upscattering
      - Considering epithermal upscattering would make it more negative
    - ENDF/B-VIII.0 may not be used for thermal reactor (PWR & BWR) analysis
  - ENDF/B release
    - May need to perform a sensitivity study for depletion effect

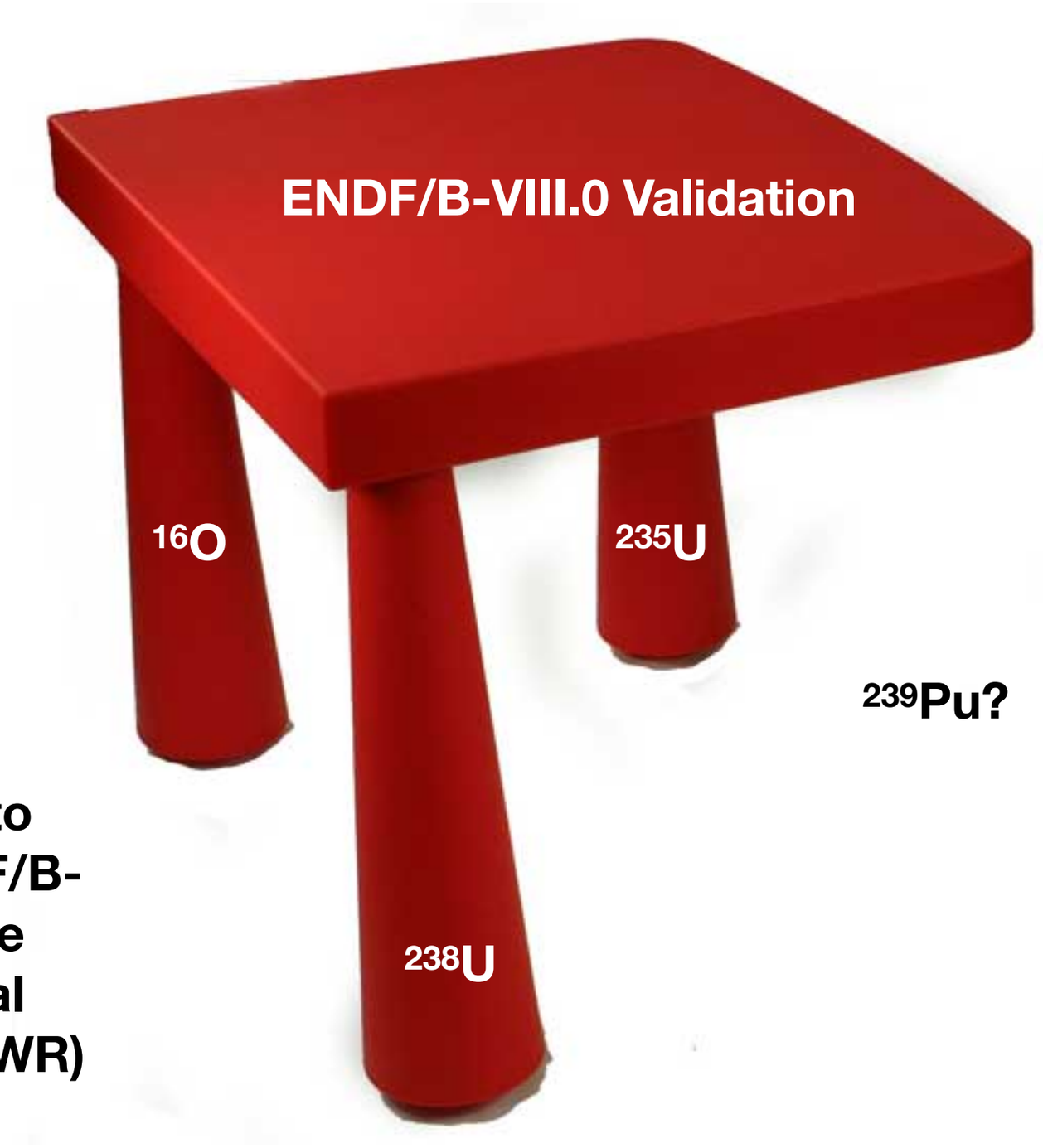
SCALE XSProc Team, CSEWG (2020)

But… We still need to re-evaluate ^{239}Pu



239Pu?

But… We still need to re-evaluate ^{239}Pu



It is premature to declare that ENDF/B-VIII.0 “cannot be used for thermal reactor (BWR & PWR) analysis”

^{239}Pu?

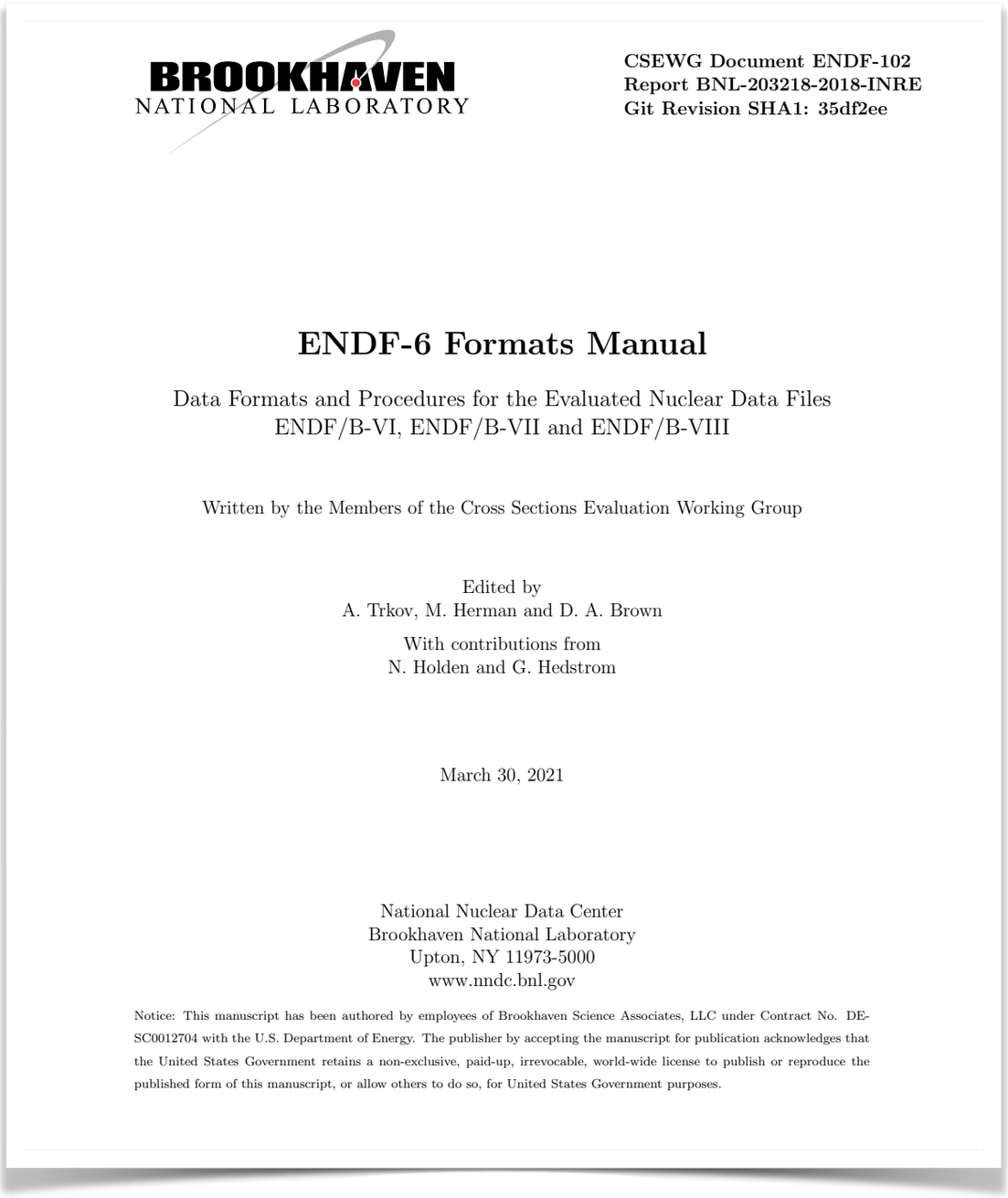
ENDF News

Two notable changes to the ENDF-6 format

ENDF/B VIII.1

- Background R-matrix
- Mixed elastic scattering in TNSL files*

* see next slide



BROOKHAVEN NATIONAL LABORATORY

CSEWG Document ENDF-102
Report BNL-203218-2018-INRE
Git Revision SHA1: 35df2ee

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown

With contributions from
N. Holden and G. Hedstrom

March 30, 2021

National Nuclear Data Center
Brookhaven National Laboratory
Upton, NY 11973-5000
www.nndc.bnl.gov

ENDF-6 Format Proposal

ENDF/B VIII.1

7.4 Mixed Elastic Scattering

Some crystalline materials have mixed coherent and incoherent elastic scattering. The coherent elastic scattering component is represented as described in Section 7.2 and incoherent elastic scattering component is represented as described in Section 7.3.

7.4.1 Formats for Mixed Elastic Scattering

The parameters to be used to calculate mixed elastic scattering are given in a section of File 7 with MT=2. The coherent elastic scattering parameters are given first followed by the incoherent elastic scattering parameters. The following quantities are defined:

ZA, AWR Standard charge and mass parameters.

LTHR Flag indicating which type of thermal data is being represented. LTHR=3 for mixed coherent and incoherent elastic scattering.

T_i Temperature (K).

LT Flag for temperature dependence. The data for the first temperature are given in a TAB1 record. The data for subsequent LT temperatures are given in LIST records using the same independent variable grid as the TAB1 record.

LI Flag indicating how to interpolate between the previous temperature and current temperature. The values are the same as for INT in standard TAB1 records.

NR, E_{int} Standard TAB1 interpolation parameters. Use INT=1 (histogram).

NP Number of Bragg edges given.

SB characteristic bound cross section (barns)

NT Number of temperatures.

$W'(T)$ Debye-Waller integral divided by the atomic mass (eV^{-1}) as a function of temperature (K).

The structure of a section is

```
[MAT, 7, 2/ ZA, AWR, LTHR, 0,  0,  0] HEAD   LTHR=3
[MAT, 7, 2/ T0, 0.0,   LT, 0, NR, NP/ Eint / S(E,T0) ] TAB1
[MAT, 7, 2/ T1, 0.0,   LI, 0, NP,  0/ S(Ei,T1) ] LIST
  -------------------------
  <repeat LIST for T2, T3, ...TLT>
  -------------------------
[MAT, 7, 2/  SB, 0.0,    0, 0, NR, NT/ Tint / W'(T) ]TAB1
[MAT, 7, 0/0.0, 0.0,    0, 0,  0,  0] SEND
```

7.4.2 Procedures for Mixed Elastic Scattering

The coherent component to the elastic scattering cross section is easily computed from $S(E,T)$ by reconstructing an appropriate energy grid and dividing S by E at each point on the grid. A discontinuity should be supplied at each E_i, and log-log interpolation should be used between Bragg edges. The cross section is zero below the first Bragg edge.

The function $S(E,T)$ should be defined up to 5 eV. When the Bragg edges get very close to each other (above 1 eV), the "stair steps" are small. It is permissible to group edges together in this region in order to reduce the number of steps given while still preserving the average value of the cross section. Either discrete angle or Legendre representations of the angular dependence of coherent elastic scattering can be constructed. It is necessary to recover the values of $s_i(T)$ from $S(E,T)$ by subtraction.

The incoherent component to the elastic scattering cross section can be used for energies up to 5 eV. The coherent and incoherent components are then added to construct the elastic scattering cross section.

Slide from M. Zerkle CSEWG (2020)

ENDF/B
VIII.1

New evaluations

INDEN, the follow on to CIELO

ENDF/B VIII.1

- $^{16,18}O$
- $^{50,51,52,54}Cr$ - 1st INDEN paper: NDS 173 (2021)
- $^{54,56,57}Fe$ - in B8.1 phase1
- ^{55}Mn - in B8.1 phase1
- $^{28,29,30}Si$ - in B8.1 phase1
- ^{233}U
- ^{235}U
- ^{239}Pu

ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Nuclear Data Sheets

Nuclear Data Sheets 173 (2021) 1–41

www.elsevier.com/locate/nds

Newly Evaluated Neutron Reaction Data on Chromium Isotopes

G.P.A. Nobre,[1,*] M.T. Pigni,[2] D.A. Brown,[1] R. Capote,[3] A. Trkov,[4] K.H. Guber,[2]
R. Arcilla,[1] J. Gutierrez,[5] A. Cuadra,[1,6] G. Arbanas,[2] B. Kos,[4] D. Bernard,[7] and P. Leconte[7]

[1] *National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973, USA*
[2] *Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*
[3] *NAPC–Nuclear Data Section, International Atomic Energy Agency, A-1040 Vienna, Austria*
[4] *Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[5] *Gonzaga University, Spokane, WA, USA*
[6] *Nuclear Systems & Structural Analysis Group, Brookhaven National Laboratory, Upton, NY 11973, USA*
[7] *CEA/DEN/CAD/DER/SPRC/Laboratoire d'Études de Physique Centre de Cadarache, Bâtiment 230, F-13108 Saint-Paul-Lez-Durance, France*

(Received December 13, 2020; accepted January 15, 2021)

Neutron reaction data for the set of major chromium isotopes were reevaluated from the thermal energy range up to 20 MeV. In the low energy region, updates to the thermal values together with an improved R-matrix analysis of the resonance parameters characterizing the cluster of large s-wave resonances for ^{50,53}Cr isotopes were performed. In the intermediate and high energy range up to 20 MeV, the evaluation methodology used statistical nuclear reaction models implemented in the EMPIRE code within the Hauser-Feshbach framework to evaluate the reaction cross sections and angular distributions. Exceptionally, experimental data were used to evaluate relevant cross sections above the resonance region up to 5 MeV in the major ^{52}Cr isotope. Evaluations were benchmarked with Monte Carlo simulations of a small suite of critical assemblies highly sensitive to Chromium data, and with the Oktavian shielding benchmark to judge deep penetration performance with a 14-MeV D-T neutron source. A significant improvement in performance is demonstrated compared to existing evaluations.

CONTENTS

* Corresponding author: gnobre@bnl.gov

https://doi.org/10.1016/j.nds.2021.04.002
0090-3752/

https://www-nds.iaea.org/INDEN/

ENDF/B VIII.1

NNL Developed TSL Evaluations

M. L. Zerkle

CSEWG – Evaluation Committee
December 1, 2020

NAVAL NUCLEAR LABORATORY

The Naval Nuclear Laboratory is operated for the U.S. Department of Energy by Fluor Marine Propulsion, LLC, a wholly owned subsidiary of Fluor Corporation.

Slide from M. Zerkle CSEWG (2020)

12 New and Revised TSL Evaluations

ENDF/B VIII.1

Material	Evaluation	MAT	Type	Temperatures	Eval. Code	Notes
UH_3	$H(UH_3)$	9	New	293.6	LEAPR	AILD, H incoherent approx.
YH_2	$Y(YH_2)$	55	Rev	293.6,400,500,600,700,800,1000,1200,1400,1600	FLASSH	AILD, Y coherent elastic
δ-ZrH_x	$H(ZrH_x)$	5	Rev	293.6,400,500,600,700,800,1000,1200	FLASSH	AIMD, H incoherent
	$Zr(ZrH_x)$	58	Rev	293.6,400,500,600,700,800,1000,1200	FLASSH	AILD. Zr coherent elastic
ε-ZrH_2	$H(ZrH_2)$	5	New	293.6,400,500,600,700,800,1000,1200	FLASSH	AIMD, H incoherent
	$Zr(ZrH_2)$	58	New	293.6,400,500,600,700,800,1000,1200	FLASSH	AILD, Zr coherent elastic,
Be_2C	$Be(Be_2C)$	28	New	293.6,400,500,600,700,800,1000,1200,1600,2000	FLASSH	AILD, Be coherent elastic
	$C(Be_2C)$	36	New	293.6,400,500,600,700,800,1000,1200,1600,2000	FLASSH	AILD, C coherent elastic
^7LiH	$H(^7LiH)$	4	New	293.6,400,500,600,700,800	FLASSH	AILD, mixed elastic scattering
	$^7Li(^7LiH)$	21	New	293.6,400,500,600,700,800	FLASSH	AILD, mixed elastic scattering
^7LiD	$D(^7LiD)$	15	New	293.6,400,500,600,700,800	FLASSH	AILD, mixed elastic scattering
	$^7Li(^7LiD)$	22	New	293.6,400,500,600,700,800	FLASSH	AILD, mixed elastic scattering

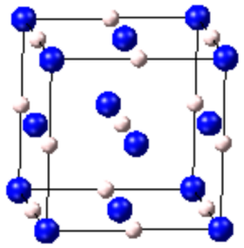
Slide from M. Zerkle CSEWG (2020)

Also have ^7LiH and ^7LiD evaluations based on incoherent approximation

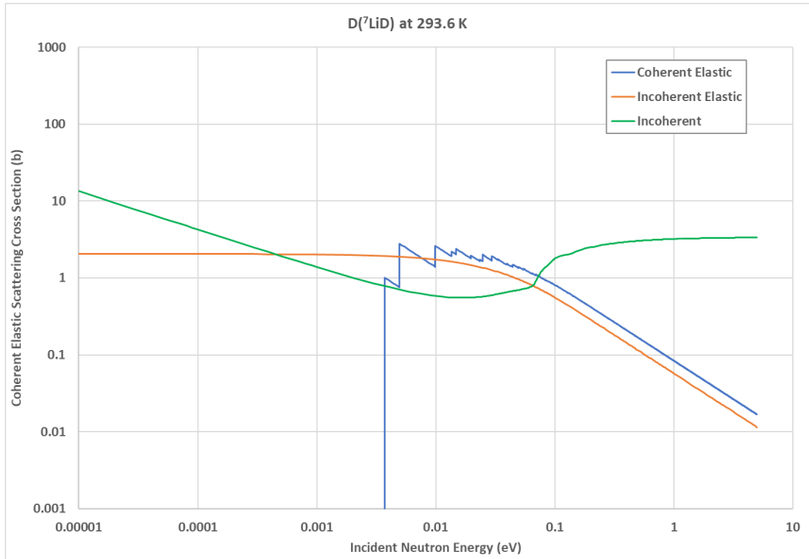
ENDF/B VIII.1

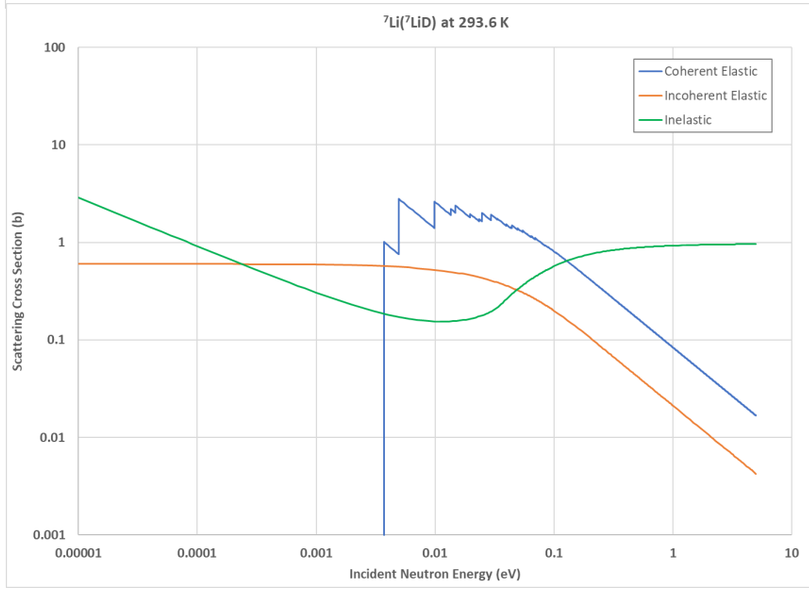
^{7}LiH and ^{7}LiD

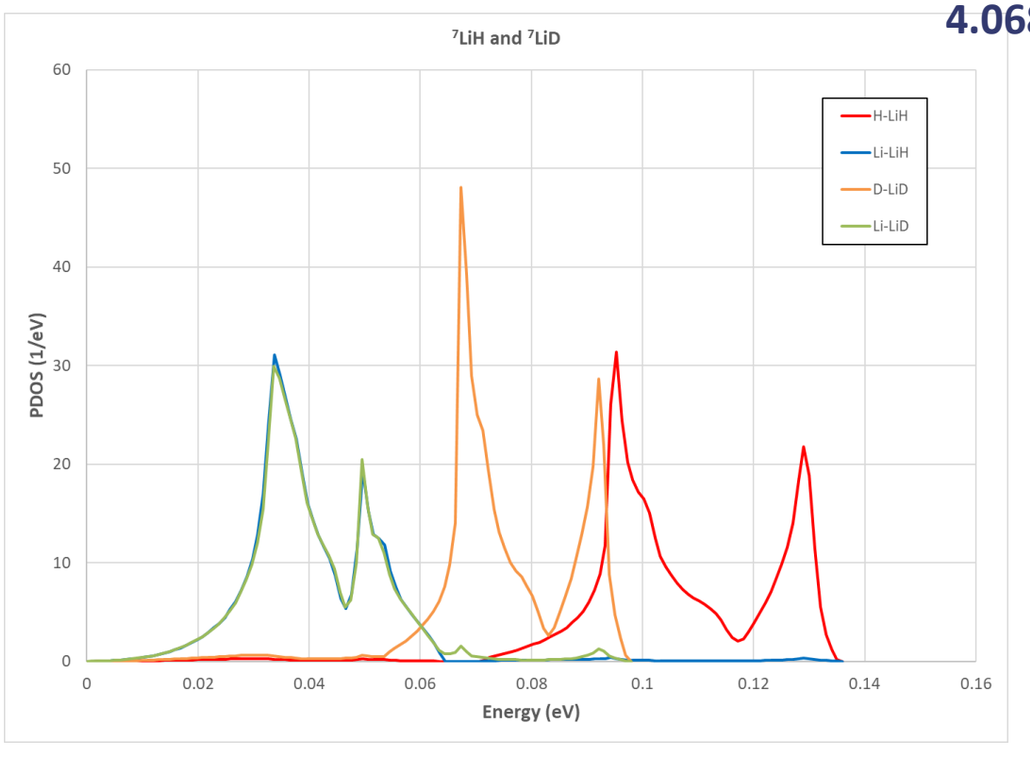
- Mixed elastic scattering treatment used to capture coherent and incoherent scattering effects in ^{7}Li and D
- AILD used to calculate PDOS
- TSL calculated at 6 temperature between 293.6 – 800 K using FLASSH
- Coherent elastic based on crystal structure and measured RT lattice constant by Zimmerman (*Phys. Rev. B*, **5**, 4704 (1972))



LiH unit cell (4.0831 Å for LiH, 4.0684 Å for LiD)



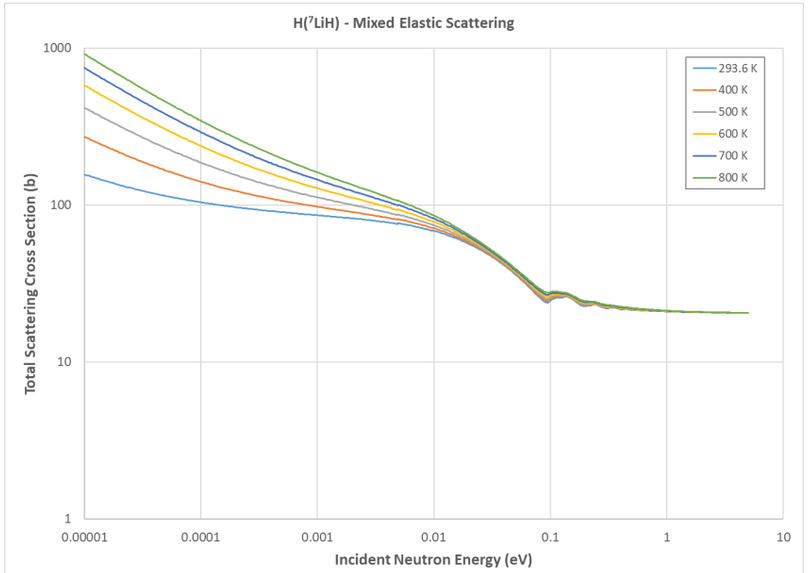


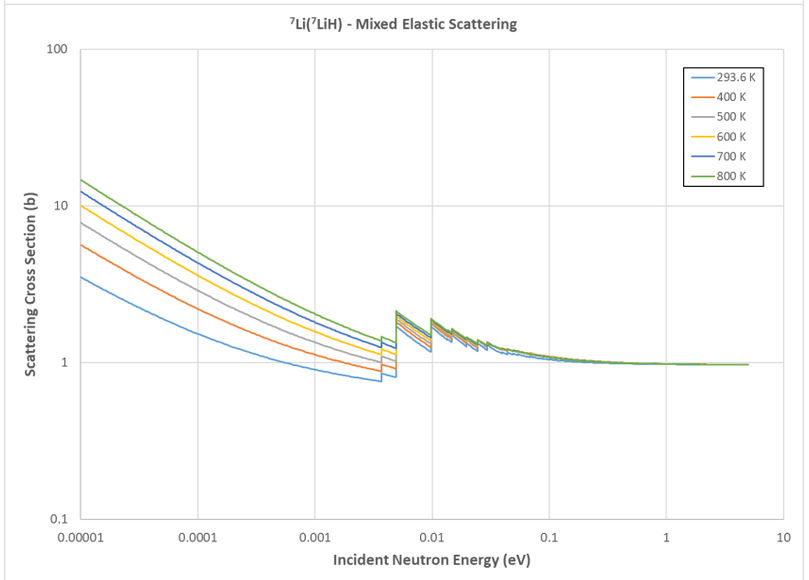


Slide from M. Zerkle CSEWG (2020)

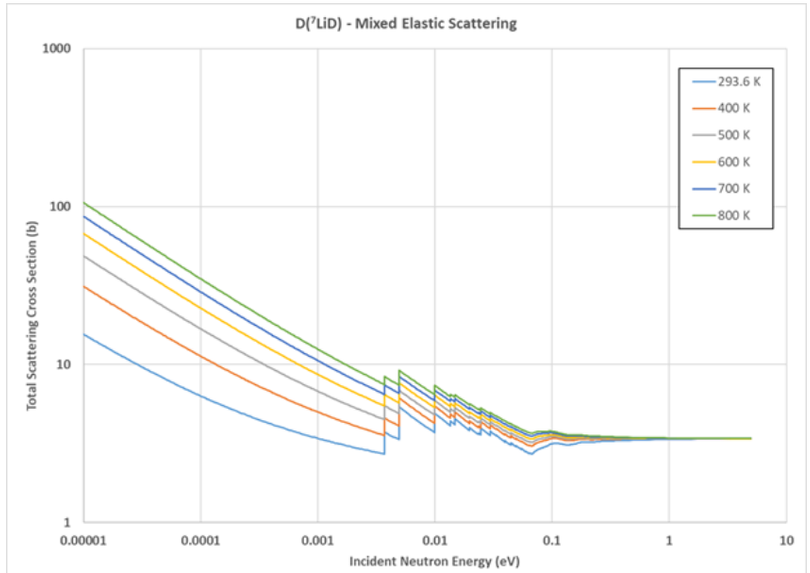
ENDF/B VIII.1

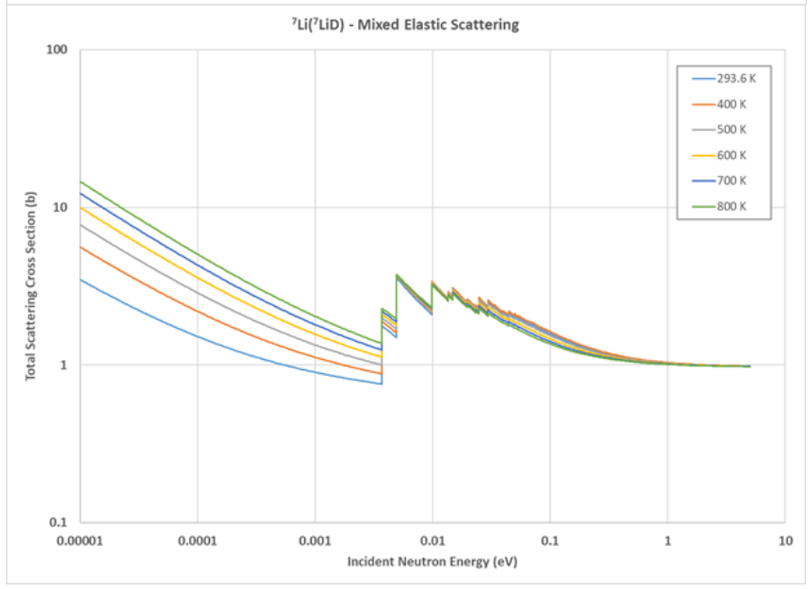
^{7}LiH





^{7}LiD





Slide from M. Zerkle CSEWG (2020)

ENDF/B
VIII.1

ENDF/B Decay Data Sub-Library

- Current version (VIII.0) current as of February 2018.
  - Decay Data Sublibrary contains spectrum data concerning nuclear decays for over 3800 isotopes (ground states and isomers).
- Version VIII.I in progress with ~435 materials updated in the last year.
- Motivation: Ensure the published ENDF/B database reflects the most current and accurate evaluations available.
- Updates:
  - Decay Half-lives for neutron rich isotopes of Z 2-28 (2015BI05).
  - TAGS spectra on $^{100,102}Nb_{gs,m}$ (2019GU03).
  - Calculated Antineutrino spectra added for neutron rich isotopes of Z 27-64.
    - Calculation made from summation beta spectra.

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BROOKHAVEN NATIONAL LABORATORY

R. Lorek CSEWG (2020)

Other improvements

ENDF/B VIII.1

Submitted

- Revised atomic libraries (D.E. Cullen, retired)
- Minor actinide nubars (R.Q. Wright, retired)
- Many fixes (R.Q. Wright, retired)
- Adopted IAEA Photonuclear Library
- Reviewing JEFF-3.3 TNSL evaluations

In preparation

- ^{239}Pu intermediate structure (M. Pigni, ORNL)
- ^{35}Cl (ORNL, LANL, LBNL)
- ^{238}U(n,n') (BNL, LBNL, LANL, LLNL)
- ^{86}Kr (BNL, NNL, MSU)
- ^{181}Ta (NNL, LANL)
- ^{140,142}Ce, ^{63,65}Cu (ORNL)
- Pb isotopes (P. Brain, RPI)
- FPY (LANL, BNL)

ENDF/B-VIII.1 Planned for Early 2023

ENDF/B VIII.1

- Target date is Feb 2023
- No change to Nuclear Data Standards, so will be called VIII.1
- “Usual” amount of changes to neutron sub library
- Substantial changes to libraries other than the neutron sublibrary: TNSL, Decay, Alpha, Photonuclear
- “Big paper” due about same time as release, to be published in Nuclear Data Sheets
- To be released in ENDF-6 and GNDS formats

ENDF-Adjacent News

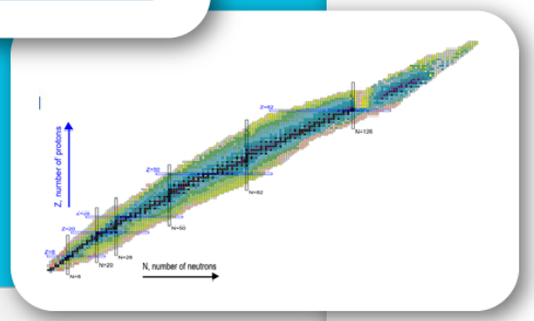
NNDC Changes

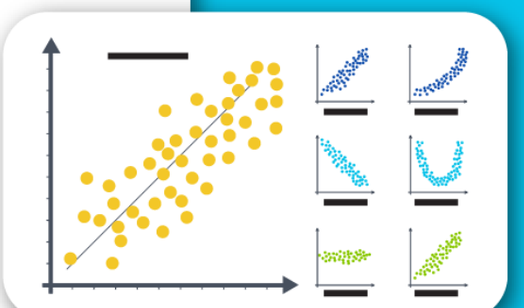
- On June 1st, I become the National Nuclear Data Center Group Leader
    - Therefore I also will chair CSEWG
    - and chair WPEC
    - and chair the US Nuclear Data Program
- Elizabeth McCutchan will be the NNDC Deputy (and next in line of succession)
- Gustavo Nobre is expected to take over as the ENDF Library Manager
- I will see GNDS-2.0 through, then we'll need to select a new EG GNDS chair

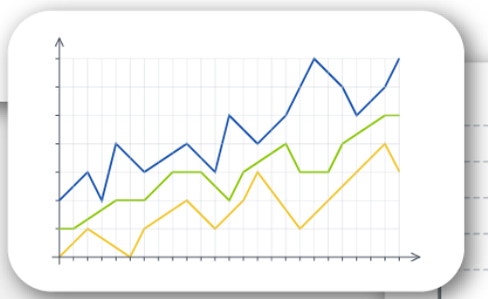
NATIONAL NUCLEAR DATA CENTER

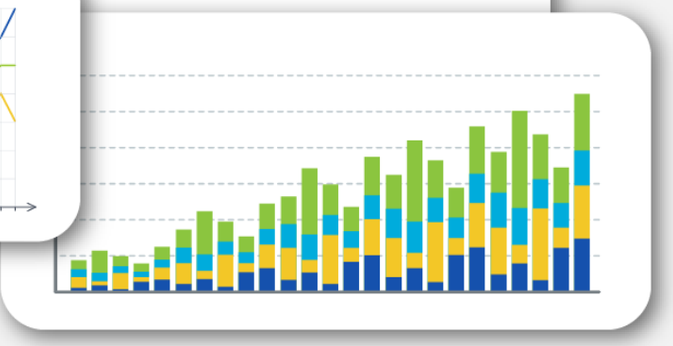
NNDC

Current, accurate, authoritative data in areas of nuclear science and engineering









PuRe Data Resources

Office of Science designated PuRe Data Resource | open data | data repositories, knowledgebases, analysis platforms

https://science.osti.gov/Initiatives/PuRe-Data

PuRe Data Resources

“The Office of Science (SC) Public Reusable Research (PuRe) Data Resources are data repositories, knowledge bases, analysis platforms, and other activities that make data publicly available to enable better communication, better stewardship, and better science.”

ENDF Implications:

- DOI’s will be generated for all ENDF datafiles
- Website will be reorganized to ensure sane DOI <-> URL mapping

Implications for other libraries:

- DOI’s will be generated for ENSDF, XUNDL, NSR datasets
- Exploring DOI generation for EXFOR