USNDP/NNDC Report

David Brown
National Nuclear Data Center

NSDD Technical Meeting
Australia National University, Canberra, Australia

Brookhaven National Laboratory
U.S. DEPARTMENT OF ENERGY
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NNDC Vision & Mission

The National Nuclear Data Center (NNDC) vision is to be the premier global resource for nuclear data and plan to:

- ❑ Implement AI/ML algorithms to reduce the time from data publication to integration in a recommended library to less than two years.
- ❑ Establish an open data repository for low-energy nuclear physics.
- ❑ Advance dissemination efforts with modern and efficient software tools.
- ❑ Sustain a robust nuclear physics research portfolio, including the development of an experimental program to accelerate isotope production science.

The NNDC is the lead and largest unit of the U.S. Nuclear Data Program (USNDP), whose mission is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. USNDP also addresses gaps in the data, through targeted experimental studies and the use of theoretical models.

National Nuclear Data Center

U.S. DEPARTMENT OF ENERGY | Office of Science

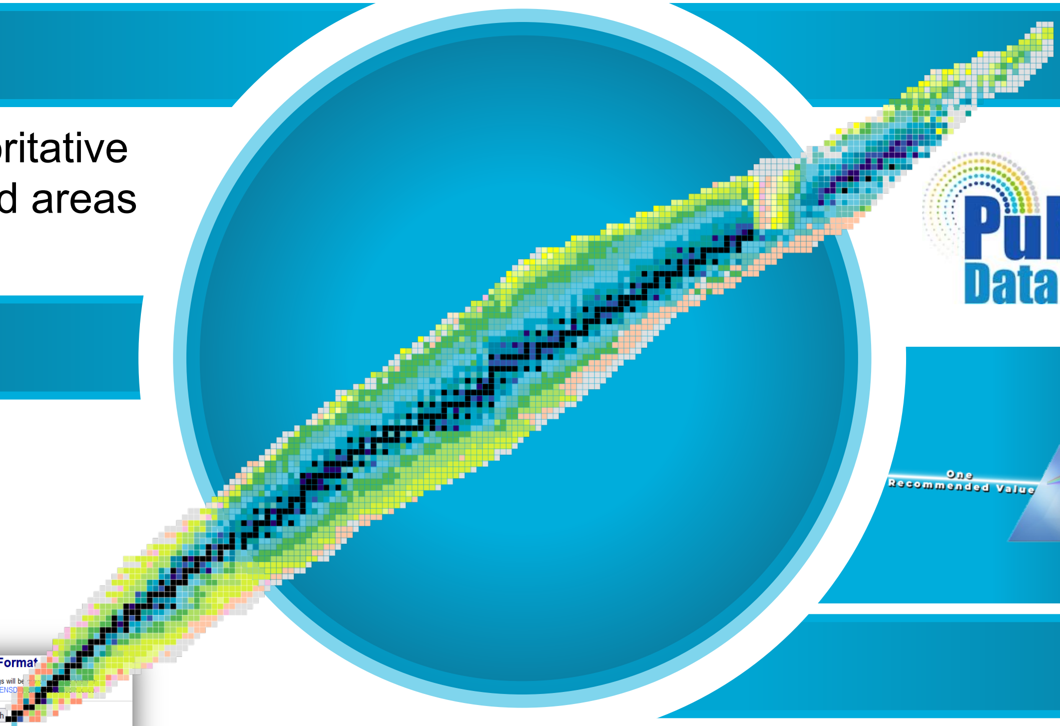
Maintaining and improving nuclear data for world-wide use

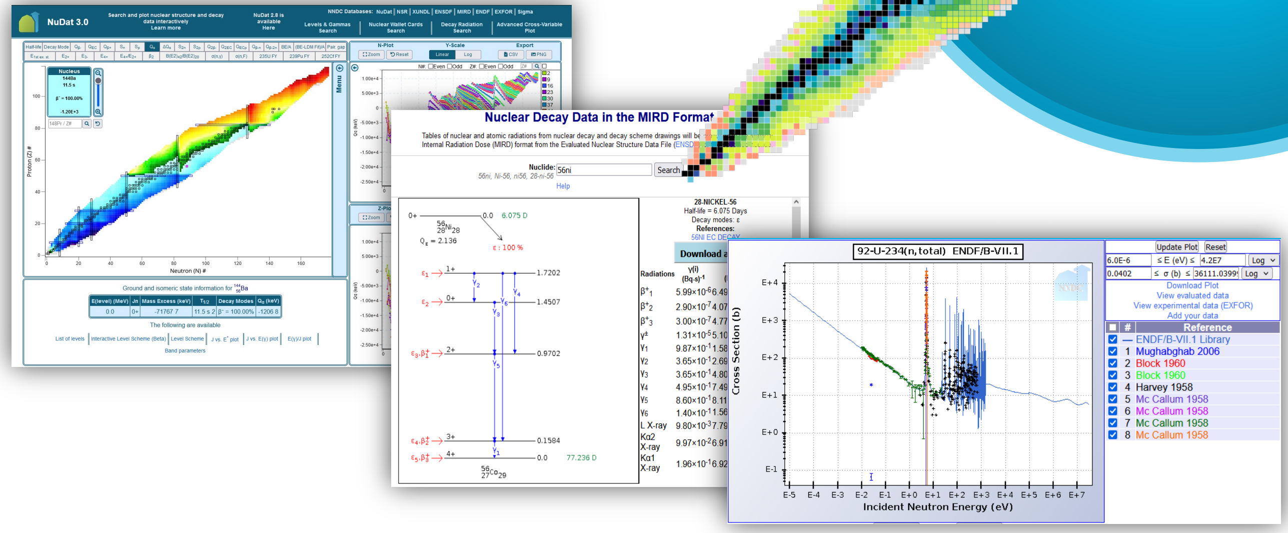
Mission

To provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering

Services

Disseminate nuclear data through feature-rich web applications





Databases

PuRe Data Resources

Nuclear Structure & Decay:

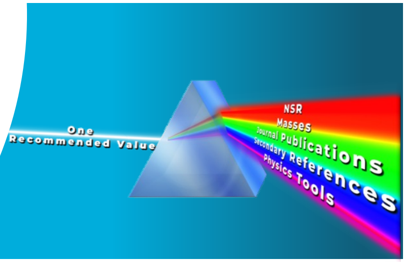
- ENSDF
- XUNDL

Nuclear Reaction:

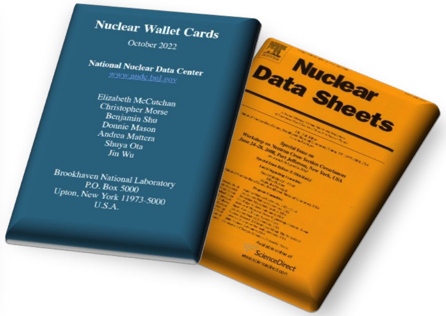
- ENDF
- EXFOR

Bibliographic:

- NSR



Publications



Nuclear Data Sheets:
World leading journal on nuclear data evaluations and research

Nuclear Wallet Cards:
Ground and isomeric state nuclear properties of all-known nuclei

National Nuclear Data Center

U.S. DEPARTMENT OF ENERGY | Office of Science

Maintaining and improving nuclear data for world-wide use

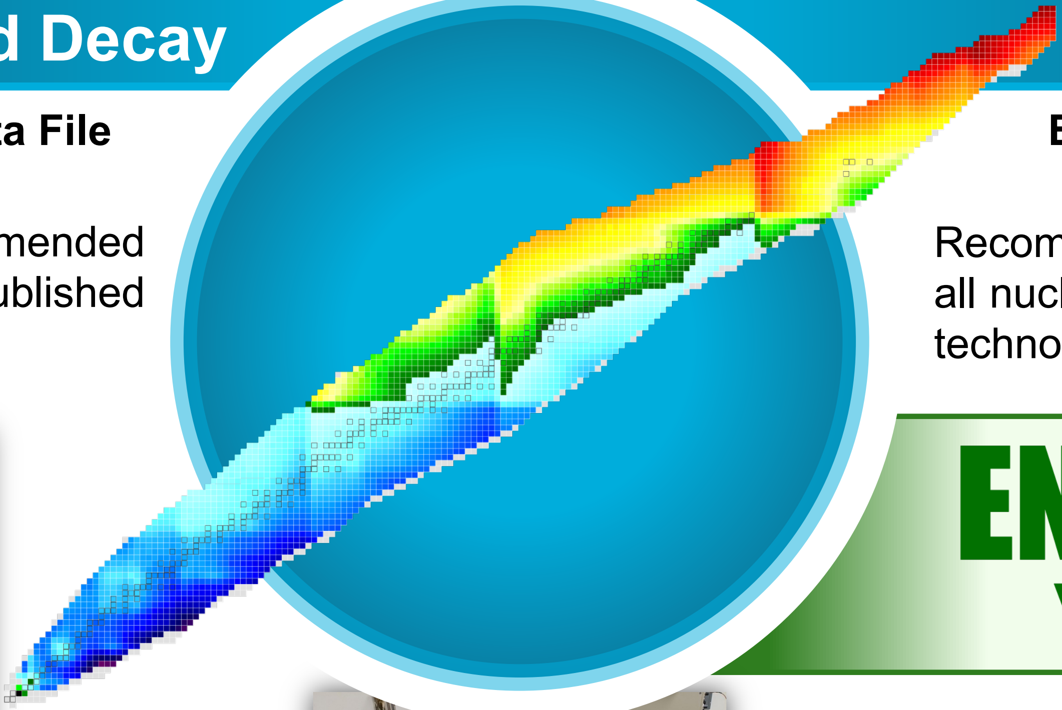
Nuclear Structure and Decay

Evaluated Nuclear Structure Data File (ENSDF)

One and only database of recommended values derived from all published experimental nuclear structure and decay data.

Experimental Unevaluated Nuclear Data List (XUNDL)

Compiled nuclear structure and decay data from recently published articles



Precision measurements of decay radiation properties

Nuclear Reactions

Evaluated Nuclear Data File (ENDF)

Recommended neutron reaction data for all nuclei relevant for nuclear science and technology

ENDF/B VIII.1

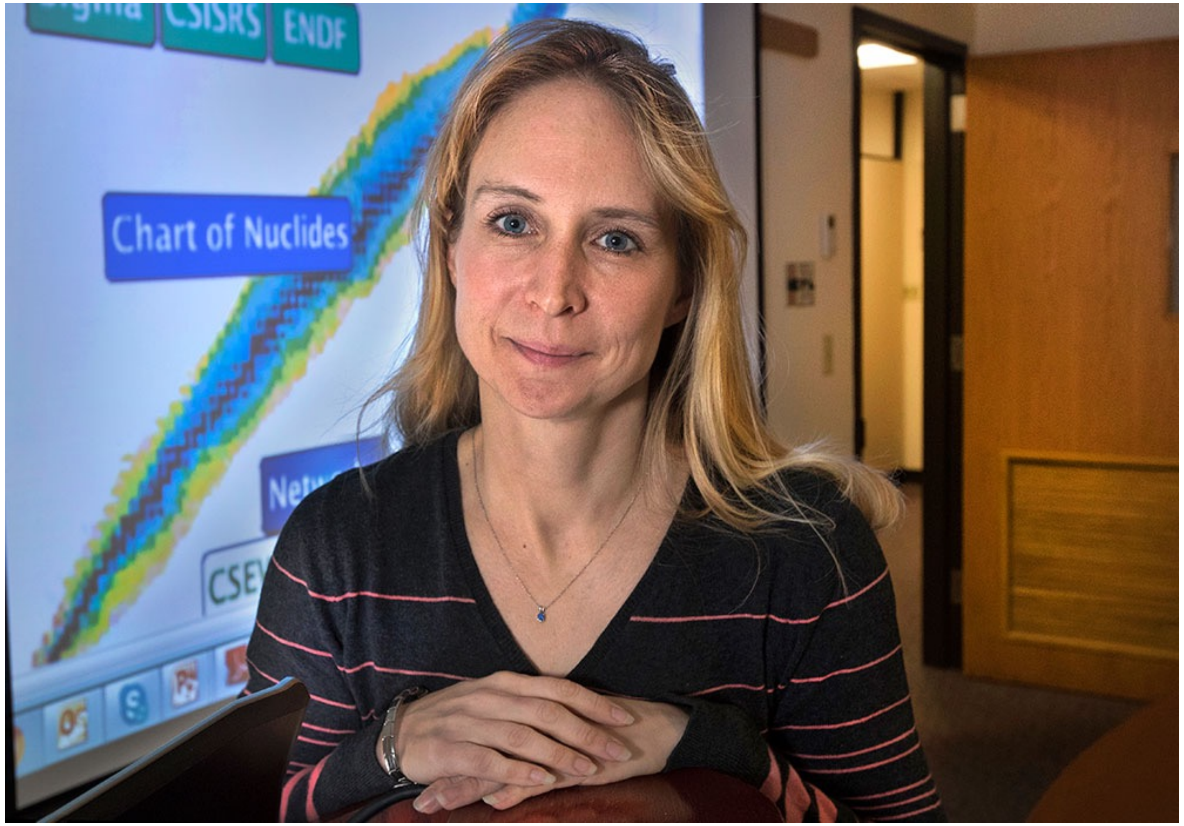
CSEWG Cross Section Evaluation Working Group

Experimental Nuclear Reaction Data (EXFOR)

World’s only repository of experimental nuclear reaction data

Elizabeth (Libby) McCutchan

- APS Fellow 2022
- Citation: *"For innovative and distinguished contributions to understanding the evolution of collectivity in heavy nuclei, critical precision experiments to test ab initio methods in light nuclei, seminal analyses of antineutrino spectra, and the development of new database tools to understand nuclear data."*



https://www.bnl.gov/newsroom/news.php?a=120865

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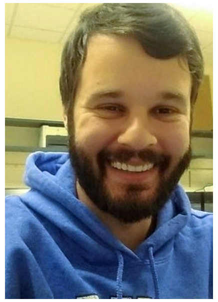
Other personnel changes at the NNDC

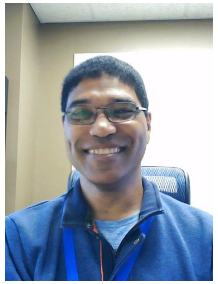
Shuya Ota joined the NNDC May 1^{st} as a scientific staff primarily working on ENSDF and XUNDL, plus developing the NNDC decay station.

Jin Wu joined the NNDC on September 6^{th} as a scientific staff working on ENSDF/XUNDL and gamma-ray spectroscopy.

Matteo Vorabbi left the NNDC Sep. 16^{th} to begin a position as Lecturer at the University of Surrey, UK.



Emanuel Chimanski joined the NNDC April 11, 2022 as a post doc working on the NA-22 Gamma Rays Induced by Neutrons project.

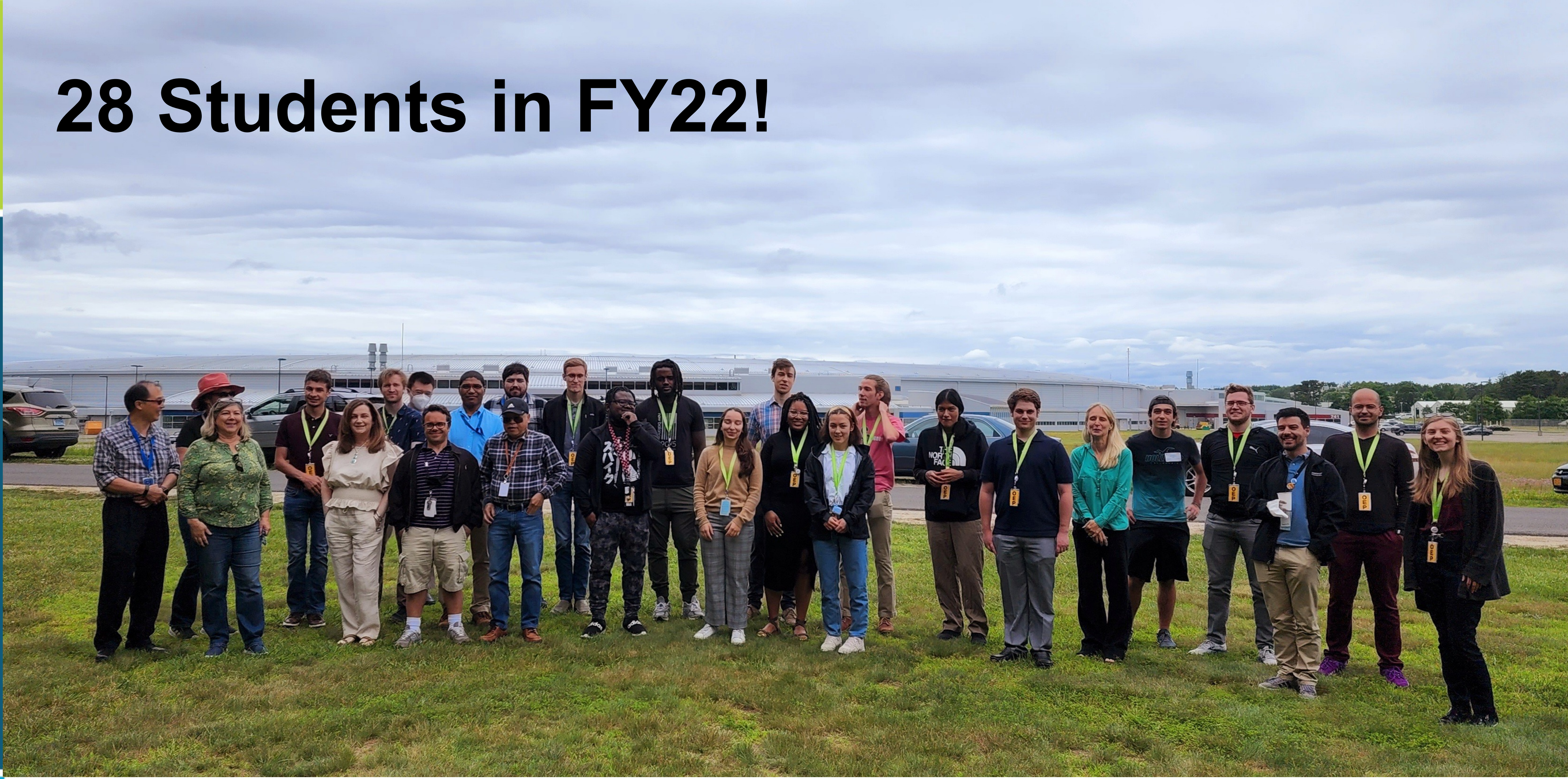


Sam Kim joined the NNDC as a post-doc on March 7^{th} to analyze data that helps determine antineutrino spectra, investigate ^{69}Ga, and experiment on ^{125}Xe trapped in silicate nanostructures.

Adam Hayes left the NNDC in January 2022 to work in the private sector

The NNDC currently has 9 staff scientists, 3 post-docs, 4 professional staff and 6 contractors

28 Students in FY22!



Half of students from traditionally underserved groups

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Nuclear Physics Traineeship allowing us to bring in URM students for longer term mentoring

Students arranged by mentor

Gustavo:
- Mary Fucci (Fall 2021 SURP)
- Ian Snider (Summer 2022 SULI)
- William “Cole” Fritsch (Summer 2022 SULI)
- Ethan Richards (Fall 2022 SULI).

Matteo:
- Khadim Mbacke (2022 NPT)
- Marcus McLaurin (2022 NPT)

Amber:
- Thomas Christo (CCI),
- John Pedersen (GRIP)
- Christian Stanley (Summer 2022 SURP)

Ben:
- Melissa Wissman (Summer 2021 SULI)

Libby:
- Grace Farrell (2022 NPT)
- Sophia Balderrama (Fall 2021, Summer 2022 SURP)
- Noah Cabanas (Fall 2021 SULI, Summer 2022 SURP)
- Meg Wynne (Spring 2022 SULI)
- Brandon Taylor (Spring 2022 SULI)
- Caroline Esposito (NPT)

Andrea:
- Sam Benda (Summer 2022 SULI)
- Mohammad Jian Najar (Summer 2022 SULI)
- Jacob Henry (Fall 2022 SULI)

Dave:
- Maxwell Rothman (Summer 2022 SULI)
- Roshen Ramnarine (Summer 2022 HSRP)

Alejandro:
- Zharia Harris (Summer 2022 SULI)
- Becket Hill (Summer 2022 SULI)
- Bryan Palaguachi (Summer 2022 SULI)
- Mathew Seeley (Summer 2022 SULI)

Arantxa:
- Caroline Sears (Summer 2022 SULI)
- Michael Romano (Summer 2022 SULI)
- Eric Schess (Summer 2022 SULI)

Donnie:
- Jada Perryman (Summer 2021 SULI)
- Edwin Gomez (Spring 2021 SULI)

Postings postings postings

Apply Now

Scientist - Nuclear Reaction Modeling & Evaluation

Job ID: 3439
Date posted: 10/27/2022

Brookhaven National Laboratory (www.bnl.gov) delivers discovery science and transformative technology to power and secure the nation's future. Brookhaven Lab is a multidisciplinary laboratory with seven Nobel Prize-winning discoveries, 37 R&D 100 Awards, and more than 70 years of pioneering research. The Lab is primarily supported by the U.S. Department of Energy's (DOE) Office of Science. Brookhaven Science Associates (BSA) operates and manages the Laboratory for DOE. BSA is a partnership between Battelle and The Research Foundation for the State University of New York on behalf of Stony Brook University. BSA salutes our veterans and active military members with careers that leverage the skills and unique experience they gained while serving our country. Our organization fully supports service members transitioning from active duty to civilian life and pledge's our commitment to actively hire veterans of the U.S. Armed Forces. Military personnel who have been formally trained or have relevant experience obtained while in service may meet educational requirements and are encouraged to apply for job opportunities at BSA.

Organizational Overview

Brookhaven National Laboratory's Nuclear Science and Technology Department conducts research and development related to nuclear technologies (reactors and accelerator-driven systems), reliability and risk assessment, and advanced modeling techniques for reactor simulation and energy systems.

The Department serves as a resource in these and related areas to support the missions of the Department of Energy (DOE), the Nuclear Regulatory Commission (NRC), and other national and international organizations. With a world-class staff of professionals with expertise in a broad range of areas related to the design and analyses of commercial, research and advanced nuclear systems, Brookhaven's capabilities and facilities are also available to support and execute experiments in support of these missions. The National Nuclear Data Center (NNDC), a part of BNL's Nuclear Science and Technology Department, is the lead unit of the US Nuclear Data Program (USNDP), whose mission is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. USNDP also addresses gaps in the data, through targeted experimental studies and the use of theoretical models.

The NNDC is responsible for the Nuclear Science Reference (NSR), eXperimental Unevaluated Nuclear Data List

What We Do

Explore career opportunities at Brookhaven Lab, where we strive to ensure the nation's security and prosperity through transformative science and technology solutions.

Research Facilities

Our world-class research facilities include:

Relativistic Heavy Ion Collider

National Synchrotron Light Source II

Center for Functional Nanomaterials

NASA Space Radiation Laboratory

Computational Science Center

https://jobs.bnl.gov/job/upton/scientist-nuclear-reaction-modeling-and-evaluation/3437/38780482704

2 staff scientists

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What we’re up to

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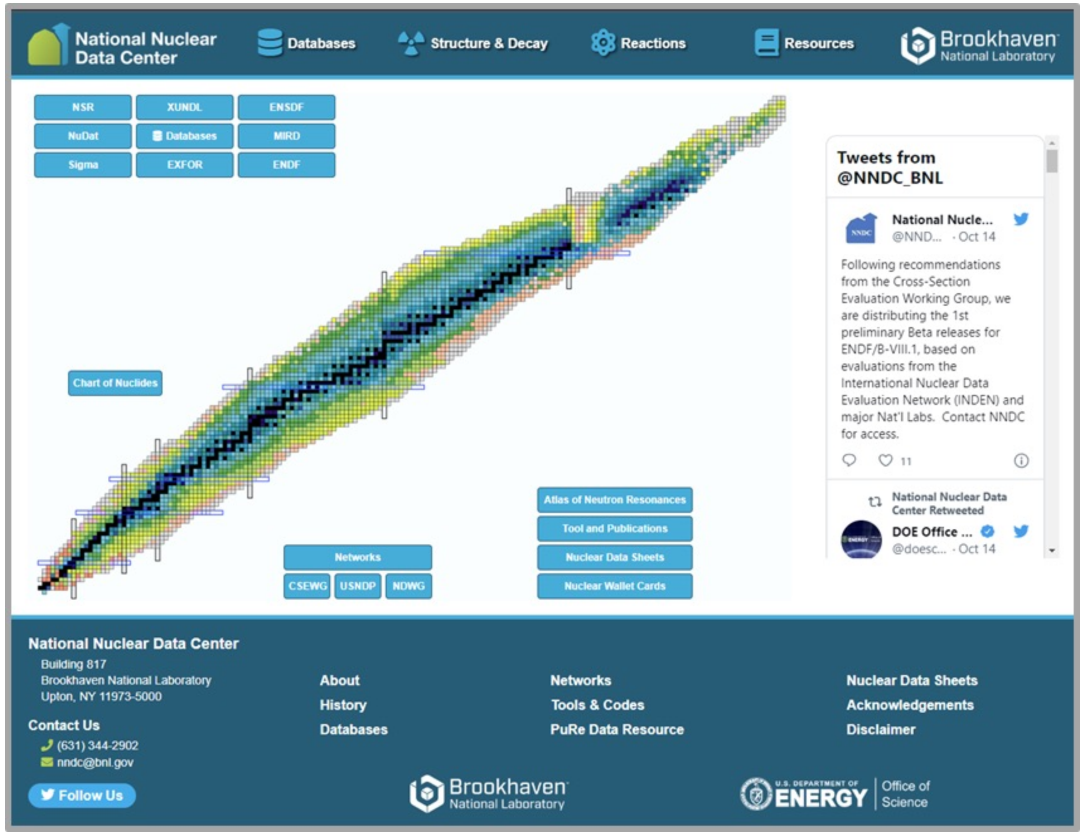
Website Redesign

- New front page + header/footer
  - Deployed in time for ND2022
  - Reduced clutter to direct users to most-trafficked websites
  - Quick access to databases
  - Use of common stylesheets for consistent design
- Roughly 80% of site fully converted to new style; all pages have new header/footer



Credit: Donnie Mason

Web Development Progress

Gradual modernization of NNDC websites

- Gradle Build Tool
  - Cross-platform development
  - Used in **54/61** websites
- GitLab CI/CD
  - Automated testing and deployment
  - Used in **36/61** websites

Allows rapid, robust web development

Web App Containers

docker

podman

Deployment of websites using Docker/Podman

- **[GOAL]:** Improve stability for web services
  - Containers can be updated/restarted individually
  - If one container crashes, the others stay up
  - In case of server failure, redeploy elsewhere
- Tests successful for **44/61** websites

Assures a secure and reliable website consistent with modern webserver practices

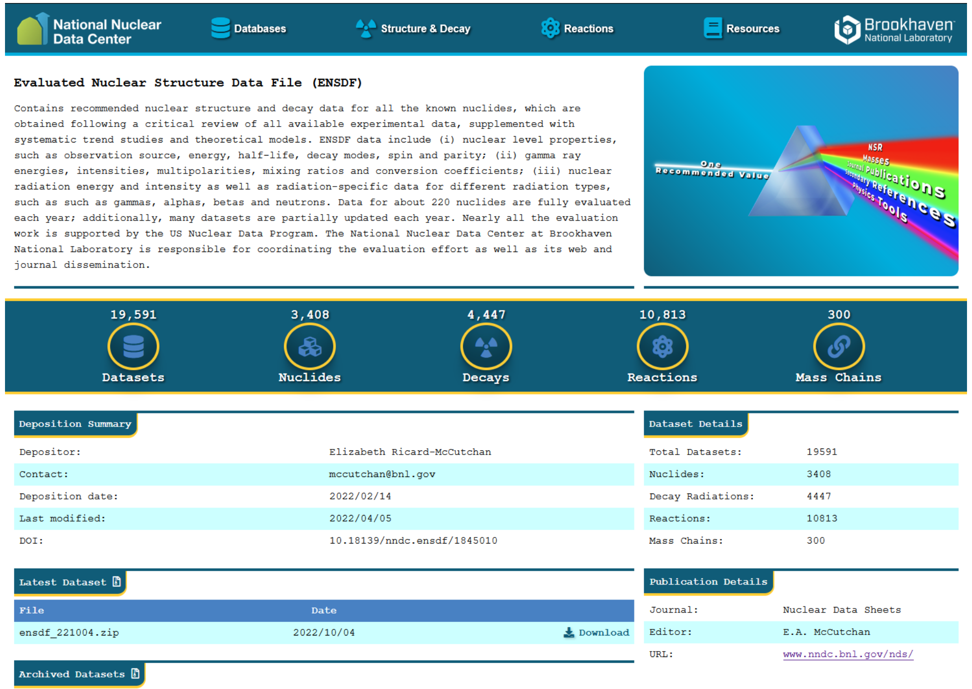
Digital Object Identifiers (DOIs)

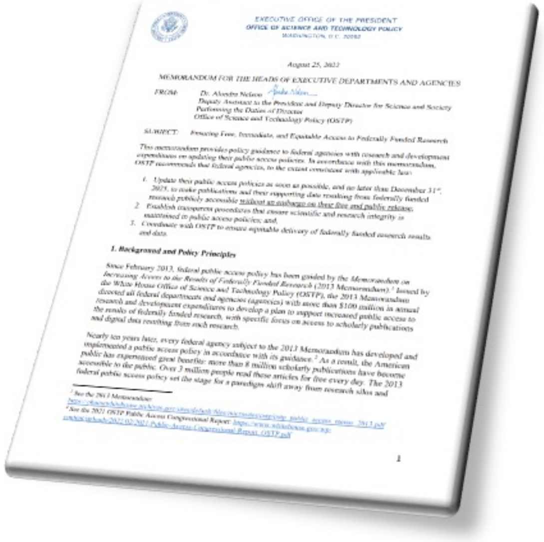
As a **Public Reusable Research (PuRe) Data Repository** the NNDC strives to make data publicly available to advance scientific knowledge

3 major libraries already have library-wide DOIs:

- ENSDF
- XUNDL
- NSR

ENDF is next!





Compliance with OSTP policy guidelines from 25 August 2022 memo

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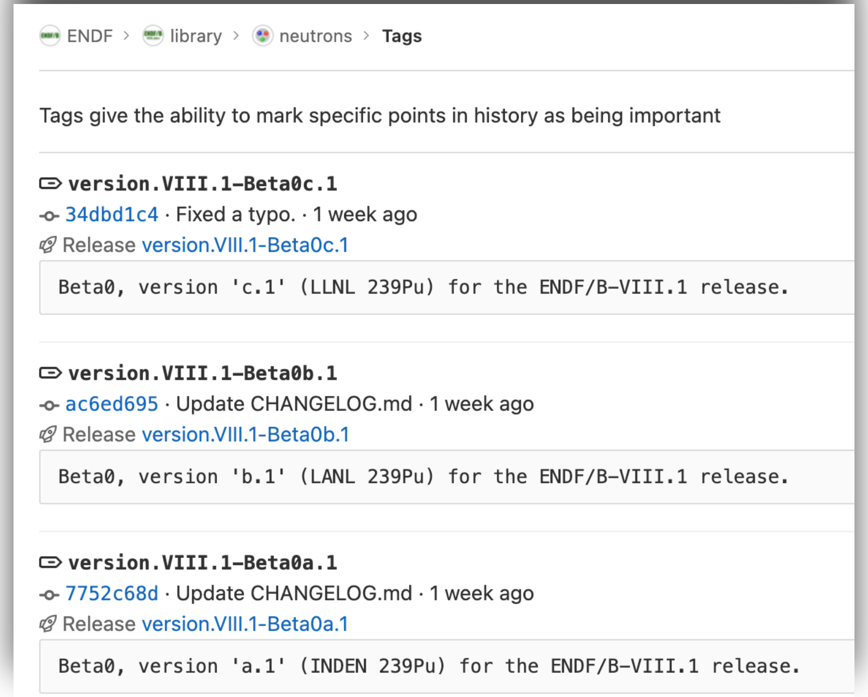
ENDF/B
VIII.1

ENDF/B-VIII.1 Beta0 released

- Needed a Beta version for preliminary validation ahead of 2022 CSEWG
- No time yet for full review: Focused on neutron sub library and materials from INDEN collaboration (some degree of internal review)
- Indicate what should be the general trend of the VIII.1 release
- 3 “sub-releases”: Different 239Pu candidates
- Planned Beta1:
  - December 2022
  - Single Pu file
  - Fully reviewed files
  - All sub libraries



Changes* in VIII.1 Beta0 from VIII.0:

- $^{28,29,30}Si$
- $^{50,52,53,54}Cr$
- $^{54,56,57}Fe$
- $^{63,65}Cu$
- $^{233,235,238}U$
- ^{239}Pu
  - Beta0a: INDEN
  - Beta0b: LANL
  - Beta0c: LLNL

**There were additional changes done shortly after the VIII.0 release, but before the whole evaluated file repository was migrated to GitLab, which are now part of ENDF/B-VIII.1Beta0:*

- ^{10}B: ENDF/B-VIII.0 errata
- $^{156,158,160,161,162,163,164}Dy$: Set of ORNL evaluations
- ^{192}Pt: Tweaked energy of first resonance
- ^{240}Pu: Fix of unitarity issue by LANL

XUNDL/ENSDF Metrics – for FY22

XUNDL

Compiler	Papers	Datasets
Shaofei	9	16
Libby	162	293
Shuya	11	17
Jin	5	10

Total of 187 papers, 336 datasets

ENSDF

Evaluator	Mass Chain	Nuclei
Chris	251	
Libby	47 (½)	30
Shuya	47(½)	

2 Mass Chains, 30 individual nuclei

NDS publications

C. Morse, "*Nuclear Data Sheets for A=267, 271, 275, 279, 283, 287, 291, 295, 299"* NDS 182, 130 (2022)

C. Morse, "*Nuclear Data Sheets for A=269, 273, 277, 281, 285, 289, and 293"*, NDS 182, 167 (2022)

S. Zhu, "*Nuclear Data Sheets for A=236"*, Nucl.Data Sheets 182, 2 (2022)
(reviewer comments received after Shaofei's passing)

ENSDF Modernization project

Data is from 40-Calcium

DSID given as non-unique text

```
40CA    ADOPTED LEVELS, GAMMAS                                  17NDS    201702
40CA  H TYP=FUL$AUT=JUN CHEN$CIT=NDS 140, 1 (2017)$CUT=30-Sep-2015$
40CA  Q -14323.0  2815635.0 6 8328.17 2 -7039.76 3    2012WA38
40CA cQ $S(2n)=28930.52 {I20}, S(2p)=14709.51 {I20} (2012Wa38)
```

Record type written here

Lines stop at/before 80

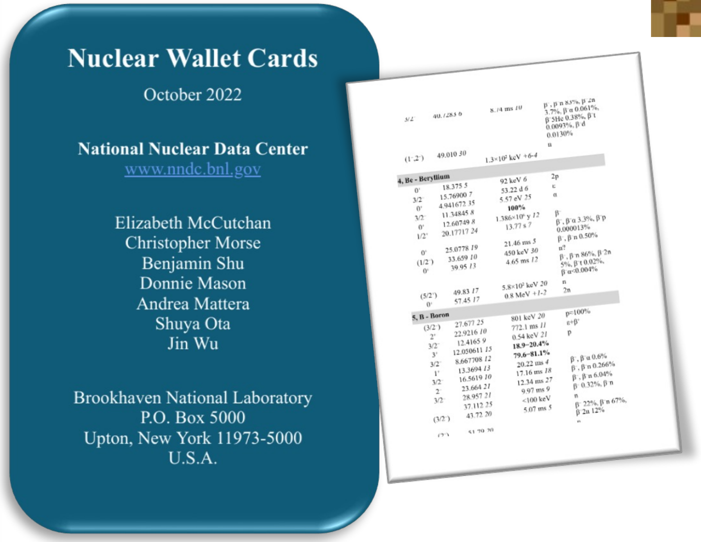
Migration from 80-column text format to object-oriented JSON-based database

- Modular, reusable design
- Labeled and formatted data can easily be parsed by both humans and computers
- Based on industry-standard technology
- JSON schema provide built-in syntax checking
  - During the migration process, this has caught many errors in the database
- Adopted and (n,γ) datasets migrated
- Currently migrating (HI,xnγ), (a,pγ), etc


```
{
    "spinParityValues": [
        {
            "spin": 2,
            "isTentativeSpin": true,
            "isTentativeParity": true,
            "parity": "+",
            "parityNumber":1
        },
        {
            "spin": 3,
            "isTentativeSpin": true,
            "isTentativeParity": true,
            "parity": "-",
            "parityNumber":-1
        }
    ],
    "comments": [
        "Assignments are based on..."
    ]
}
```

WalletCraft a new evaluation of properties of ground-state and long-lived isomers for all known nuclei

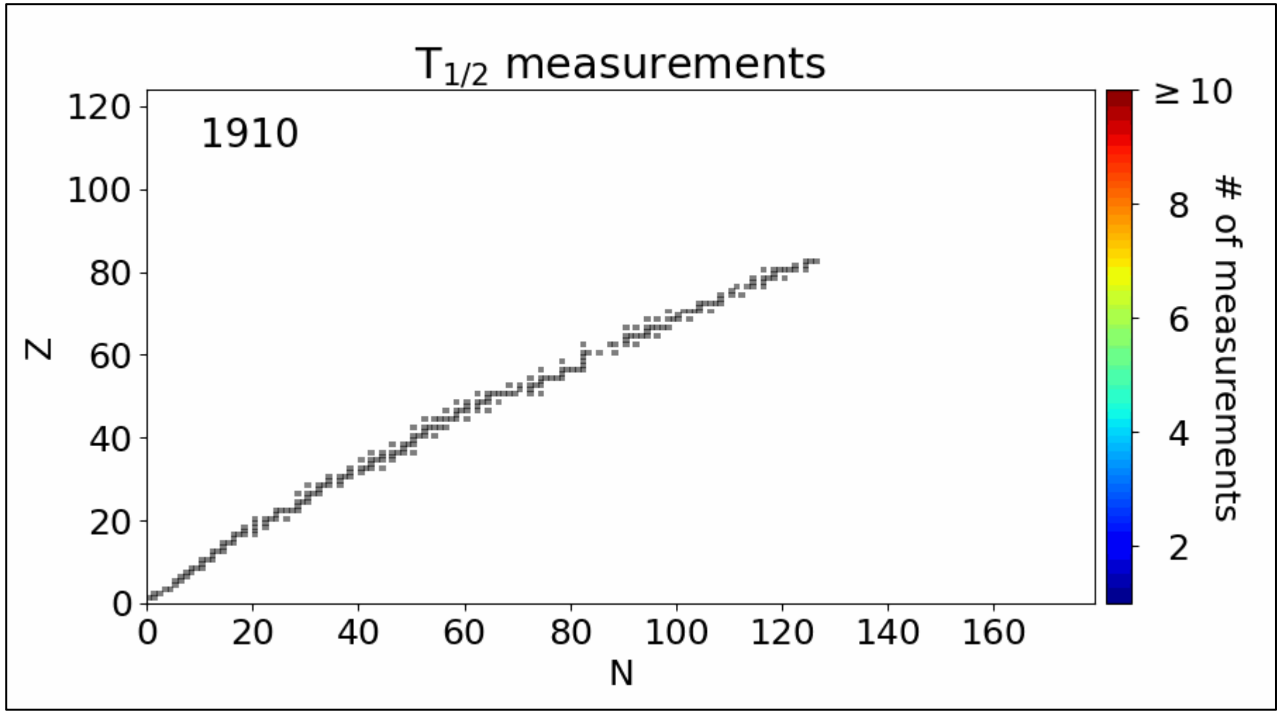
Evaluation for g.s. and isomers ($T^{1/2}$>100ms) of:
- Spin/Parity
- Mass Excess – from AME2020
- Half-life, Width or Abundance
- Decay Mode(s)



A new version of the Nuclear Wallet Cards booklet is available!

Major changes *under the hood*:
- New JSON-based OODB
- We store experimental measurements (building block of the evaluation)

Advantages:
- Transparent documentation of evaluation history
- Format can be easily read in modern codes and data plotted/analyzed
- Allows for much shorter versioning (from 5-10 yr to ~1yr)



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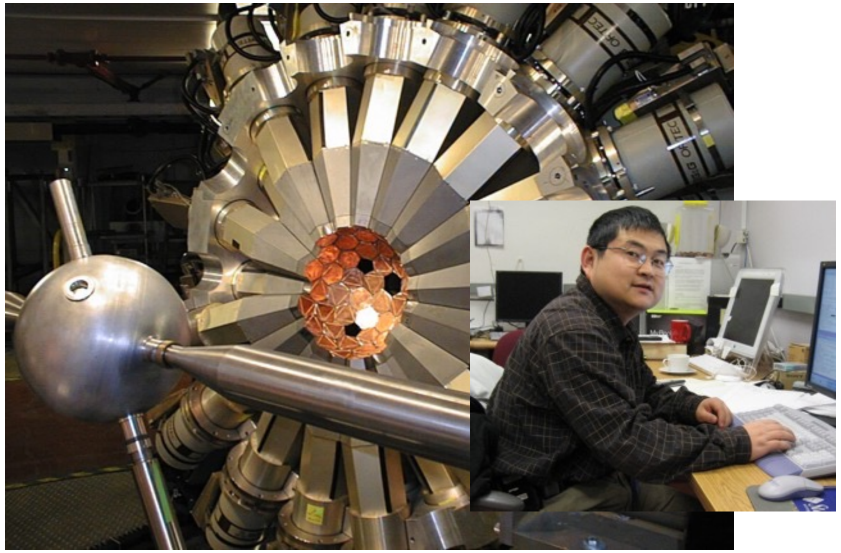
Highlights

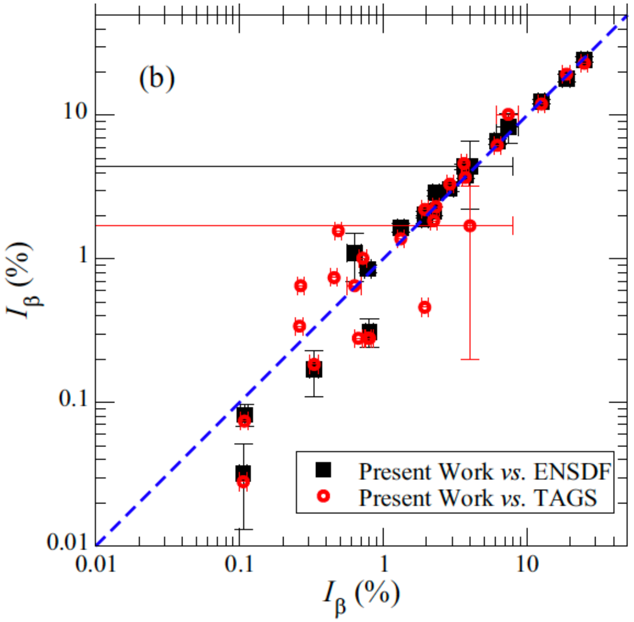
(some expected, some not!)

"Complete" spectroscopy with Gammasphere

Gammasphere at ANL



- 70 + new transitions added to the level scheme
- Excellent agreement with Greenwood TAGS – but now with uncertainties!



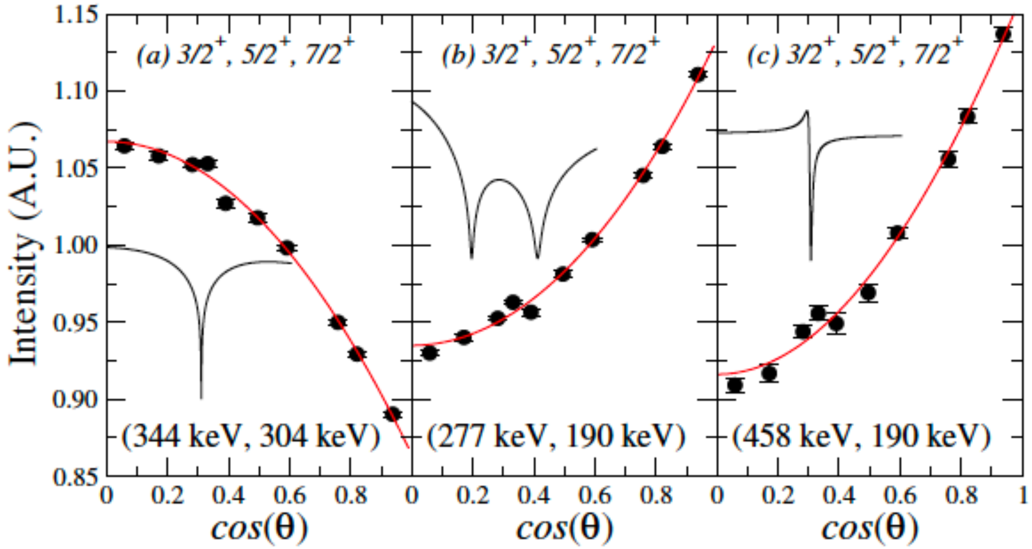
27 definite J assignments – out of 37 levels

Data from a 10 year old experiment to study Coulex of ^{141}Cs

PHYSICAL REVIEW C **106**, 034318 (2022)

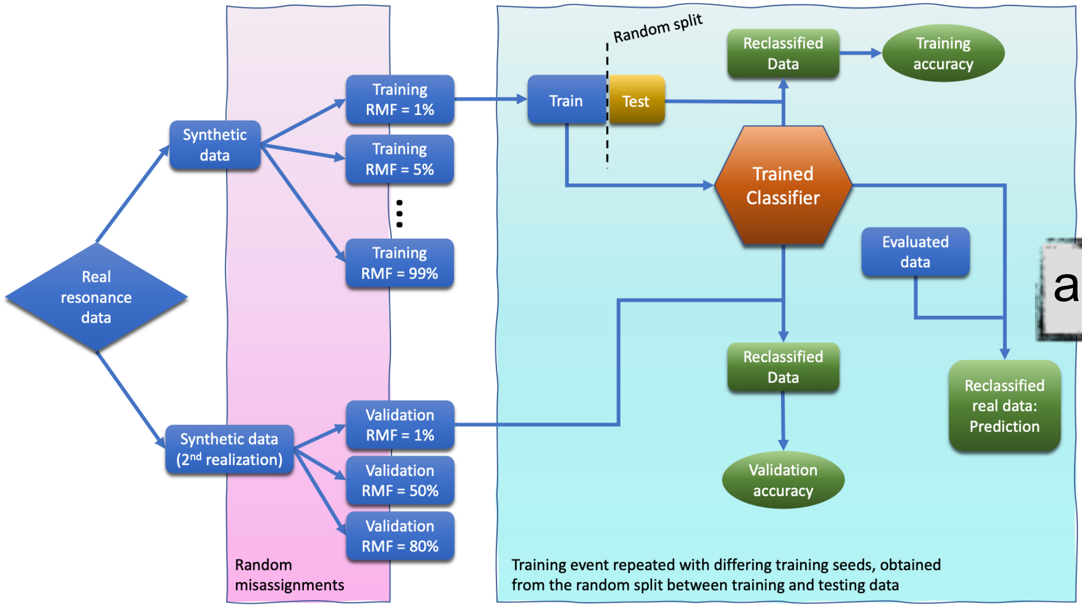
β decay of ^{141}Ba

Javier Rufino, Jr.,[1,2] E. A. McCutchan,[2] S. Zhu,[2,3] A. A. Sonzogni,[2] M. Alcorta,[3] P. F. Bertone,[3] M. P. Carpenter,[3] J. Clark,[3] C. R. Hoffman,[3] R. V. F. Janssens,[4,5] F. G. Kondev,[3] T. Lauritsen,[3]



Bayesian Resonance Reclassifier

- First paper on ML method for reclassification of neutron resonances submitted to PRC!
- Proof-of-principle, description of features
- Applied to ^{52}Cr resonances as test case



arXiv:2209.14403

arXiv:2209.14403v1 [nucl-th] 28 Sep 2022

A novel Machine-Learning method for spin classification of neutron resonances

G. P. A. Nobre* and D. A. Brown
National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA

S. J. Hollick
Department of Physics, Yale University, New Haven, CT, 06520, USA

S. Scoville
University of Pittsburgh, Pittsburgh, PA 15217, USA and
Rensselaer Polytechnic Institute, Troy, NY, 12180, USA

P. Rodríguez
Pacific Northwest National Laboratory, Richland, WA 99354, USA and
University of Puerto Rico, Mayagüez Campus, Mayagüez, 00682, Puerto Rico

(Dated: September 30, 2022)

The performance of nuclear reactors and other nuclear systems depends on a precise understanding of the neutron interaction cross sections for materials used in these systems. These cross sections exhibit resonant structure whose shape is determined in part by the angular momentum quantum numbers of the resonances. The correct assignment of the quantum numbers of neutron resonances is, therefore, paramount. In this project, we apply machine learning to automate the quantum number assignments using only the resonances' energies and widths and not relying on detailed transmission or capture measurements. The classifier used for quantum number assignment is trained using stochastically generated resonance sequences whose distributions mimic those of real data. We explore the use of several physics-motivated features for training our classifier. These features amount to out-of-distribution tests of a given resonance's widths and resonance-pair spacings. We pay special attention to situations where either capture widths cannot be trusted for classification purposes or where there is insufficient information to classify resonances by the total spin J. We demonstrate the efficacy of our classification approach using simulated and actual ^{52}Cr resonance data.

I. INTRODUCTION

Neutron scattering and reaction data for neutron energies ranging from 10^{-5} eV to 20 MeV are needed for simulations of nuclear systems in nuclear fission and fusion energy production, stockpile stewardship, non-proliferation, etc. [1]. For energies below that typical of fission neutrons, ~ 1 MeV, normally only elastic and capture (and fission for actinides) channels are open. For all but the lightest nuclei, these reaction channels all exhibit strong resonant structure that we identify with the energy levels of the compound nucleus formed by the capture of the neutron into the target state [2].

The double differential capture or elastic scattering cross sections are completely determined by the set of resonance energies, the decay widths to each of the observed reaction channels and incident neutron orbital angular momentum L and the total angular momentum J characterizing these reaction channels [1], when described using R-matrix theory [3, 4]. We cannot predict the energies and widths of the resonances in any nuclei other than the lightest systems with current theoretical and computational approaches. The resonance energies and widths must be determined by fitting experimental transmission or cross section measurements. To complicate matters, the shape of the R-matrix fitting function is heavily dependent on the quantum numbers (L, J) assigned to the particular resonance.

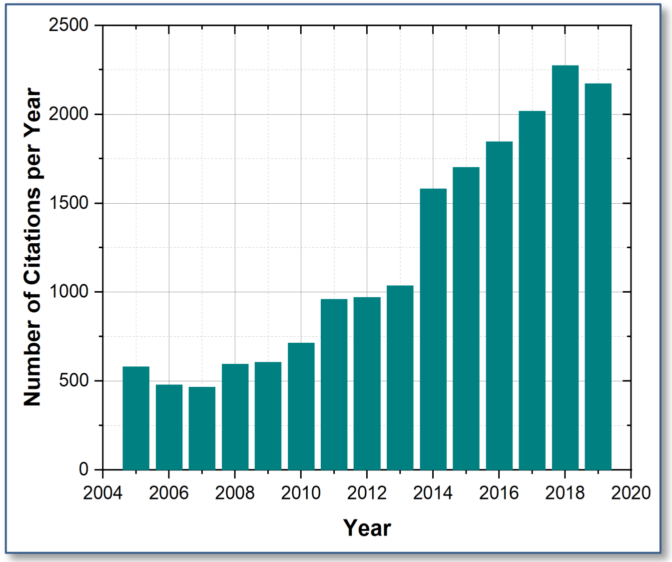
Codes, such as SAMMY [5] and REFIT [6], use a Generalized Least-Squares Fitting routine derived from a linearized version of Bayes' Equation. Conventional evaluations based on SAMMY or REFIT require significant preparation by an evaluator to establish reliable prior estimates of the widths, energies and (L, J) quantum numbers of the resonances, ensuring that one is sufficiently close to the χ^2 minimum for the fit to be well founded. Unfortunately, the shear number of known resonances in a typical evaluation makes this endeavor tedious and time-consuming. Furthermore, this step of the evaluation is subjective, relying on the experience of the evaluator and, therefore, it is hardly reproducible. This fact leads to significant amounts of unquantified uncertainty in the final evaluation.

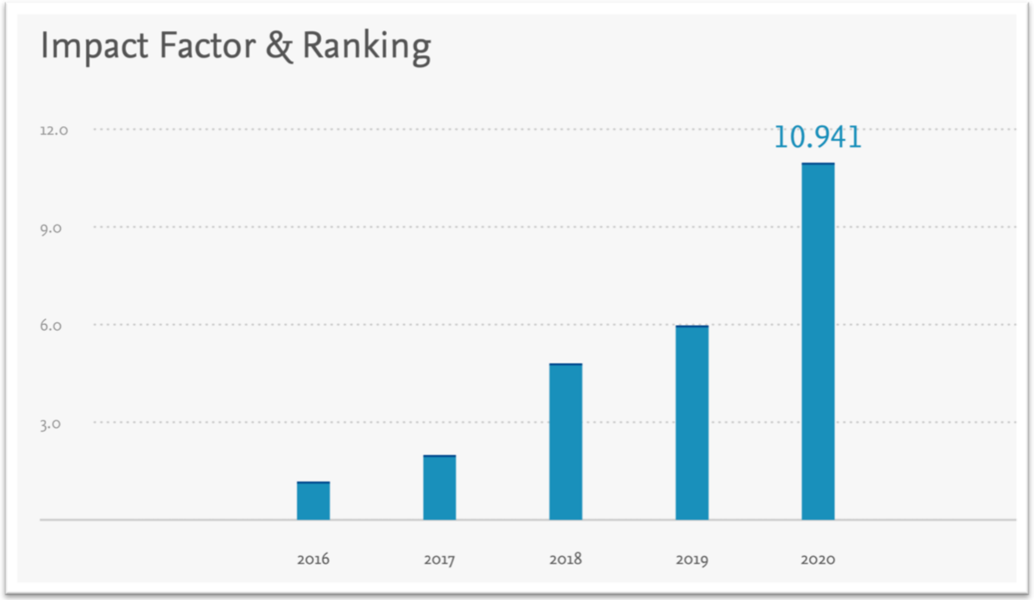
There are a number of experimental techniques that can help determine the incident neutron orbital angular momentum L and the total angular momentum J of each resonance including study of the low-energy γ-ray cascades from neutron capture events detected by Ge-Li detectors, γ-ray multiplicity methods, and measurements

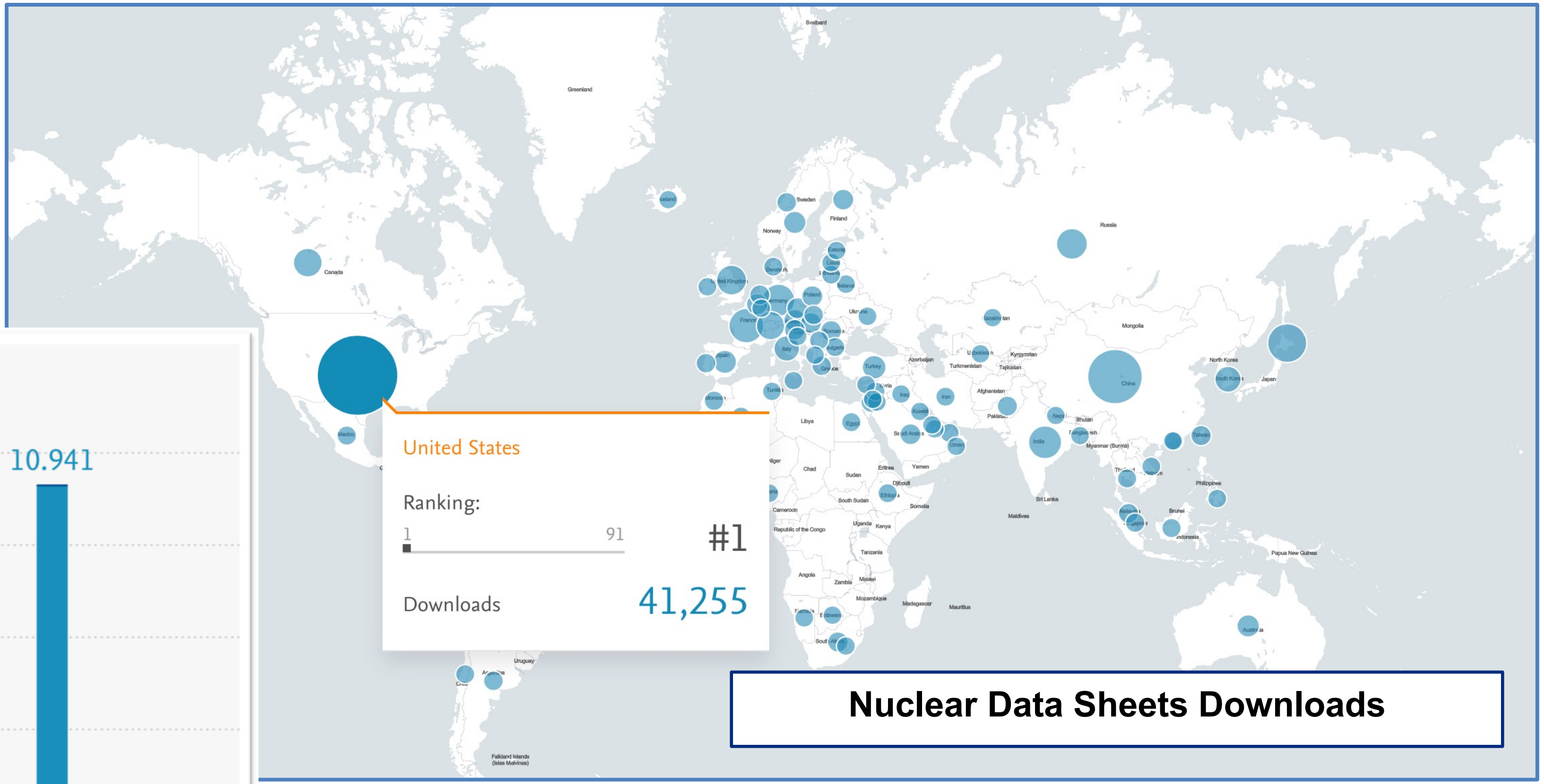
* Corresponding author: gnobre@bnl.gov

[1] In the JLS coupling scheme which we use in this work, there is also the total spin of the incident channel, S. This can usually be determined from knowledge of L and J for s- and p-wave resonances.

Nuclear Data Sheets Citations & Impact Factor







Nuclear Data Sheets Downloads

NDS > PRL!

Publications

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Publications 1/3

2022Pr08 Nucl.Phys. A1027, 122511 (2022) **B.Pritychenko**, B.Singh, M.Verpelli Systematic trends of 0+-2, 1--1, 3--1and 2+-1 excited states in even-even nuclei COMPILATION 4He,12,16O,44Ar,40Ca,68Ni,72Ge,72Kr,90,96,98Zr,98Mo,180, 182Hg,184,186,188,190,192,194Pb,14C,14O,146Gd,208Pb; analyzed available data; deduced J, pi, 2+ first excited state dominance in even-even nuclei.

2022Ze01 J.Instrum. 17, P03012 (2022) V.V.Zerkin, **B.Pritychenko, J.Totans**, L.Vrapcenjak, A.Rodionov, G.I.Shulyak EXFOR-NSR PDF database: a system for nuclear knowledge preservation and data curation

2022At03 Phys.Rev. C 105, 055503 (2022) M.Atzori Corona, M.Cadeddu, N.Cargioli, P.Finelli, **M.Vorabbi** Incorporating the weak mixing angle dependence to reconcile the neutron skin measurement on 208Pb by PREX-II **2022Vo02** Phys.Rev. C 105, 014621 (2022) **M.Vorabbi**, M.Gennari, P.Finelli, C.Giusti, P.Navratil, R.Machleidt Elastic proton scattering off nonzero spin nuclei

2022Mo05 Nucl.Instrum.Methods Phys.Res. A1025, 166155 (2022) **C.Morse**, H.L.Crawford, A.O.Macchiavelli, A.Wiens, M.Albers, A.D.Ayangeakaa, P.C.Bender, C.M.Campbell, M.P.Carpenter, P.Chowdhury, R.M.Clark, M.Cromaz, H.M.David, P.Fallon, R.V.F.Janssens, T.Lauritsen, I.-Y.Lee, C.J.Lister, D.Miller, V.S.Prasher, S.L.Tabor, D.Weisshaar, S.Zhu The polarization sensitivity of GRETINA NUCLEAR REACTIONS 24Mg(p,p'), E=2.45 MeV; measured reaction products, E gamma,I gamma. 25Mg; deduced gamma-ray energies, J, pi, polar angular distribution.

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