TSL Nuclear Fuel Evaluations and Capabilities at NC State University

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Outline

- **Provide thermal scattering law (TSL) and cross section data to support advanced reactor modeling and criticality safety**
  - **Modeling and Simulations**
  - **Uranium Fuel Materials**
  - **Evaluation Updates**
  - **Benchmark Applications**

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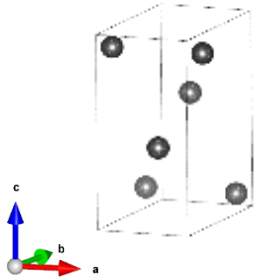
Material Modeling



Pseudo-potential

Quantum mechanical model

Optimize the system structure

Evaluate Hellmann-Feynman forces

DFT

Generate displacements

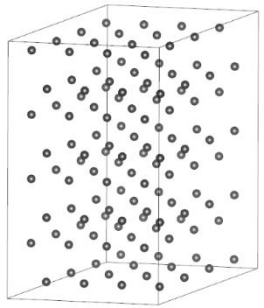
Evaluate the dynamical matrix

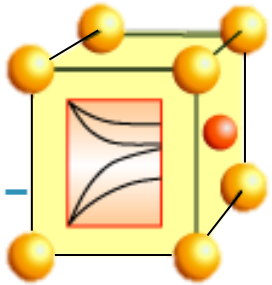
Sample the Brillouin zone

Phonon model

Harmonic potential

Lattice Dynamics





Density of states / phonon dispersion

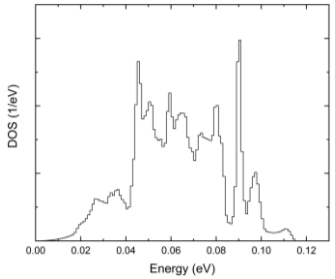
Thermal Scattering Law S(α,β)

Thermal scattering cross section

FLASSH

Phonon expansion

Temperature dependent



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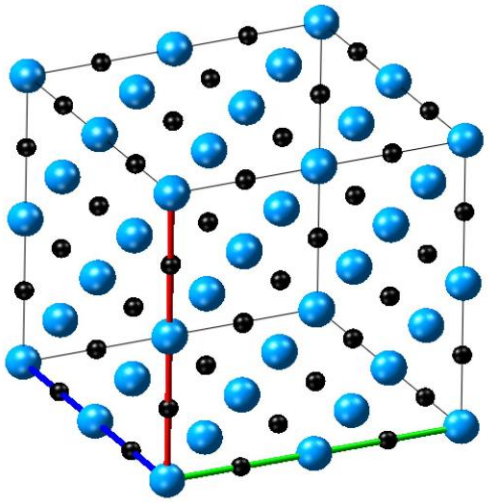
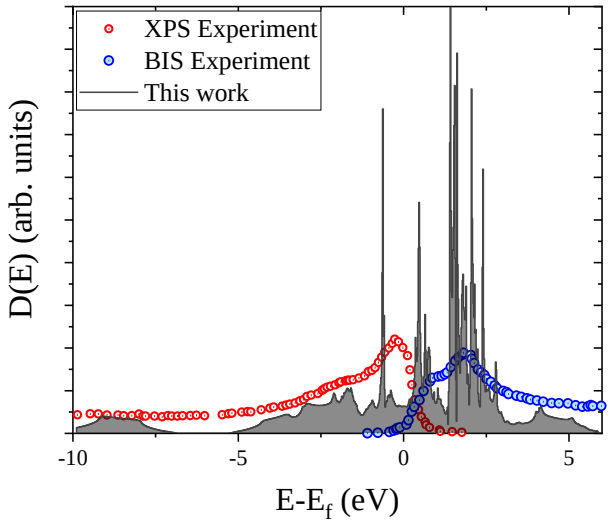
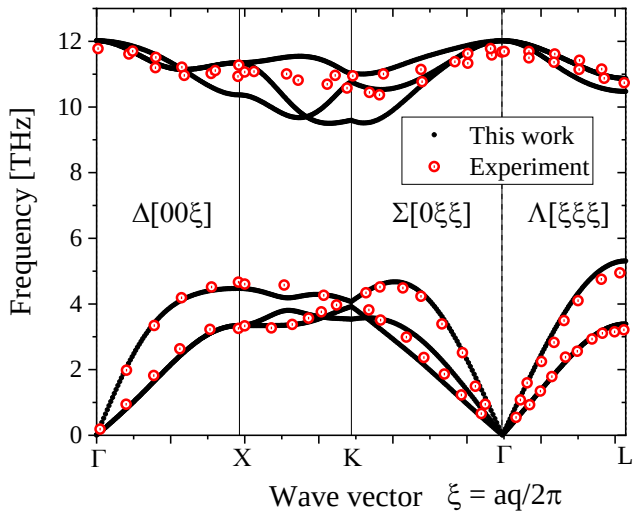
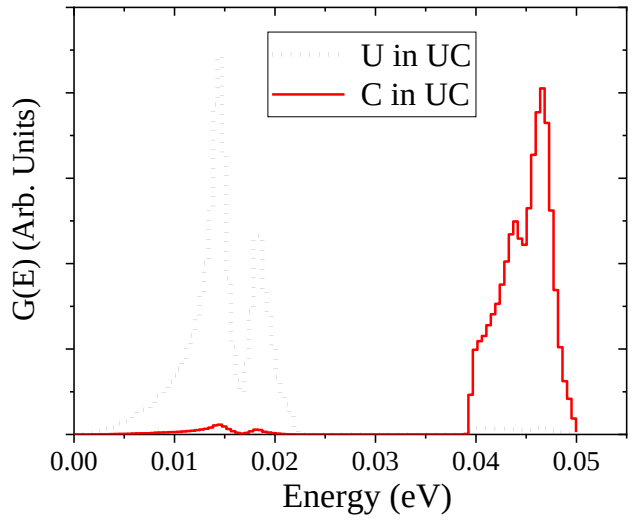
Uranium Carbide

- VASP DFT Framework
  - GGA-PBEsol Pseudopotential
  - 1.9 eV Effective Hubbard Term
  - Magnetic Structure Captured with Spin-Orbit-Coupling
    - AFM-I polarizations in x, y, z -> paramagnetic
    - 2x2x2 supercell (64 atoms)



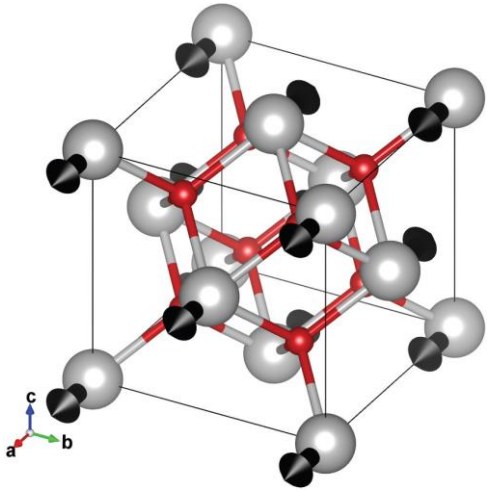


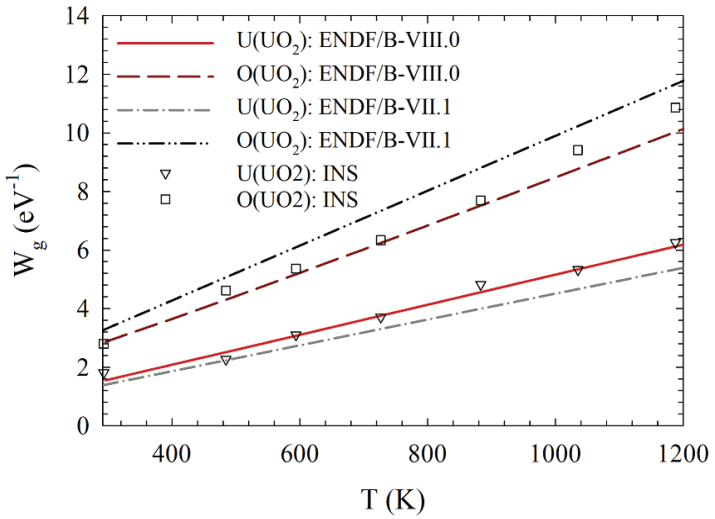


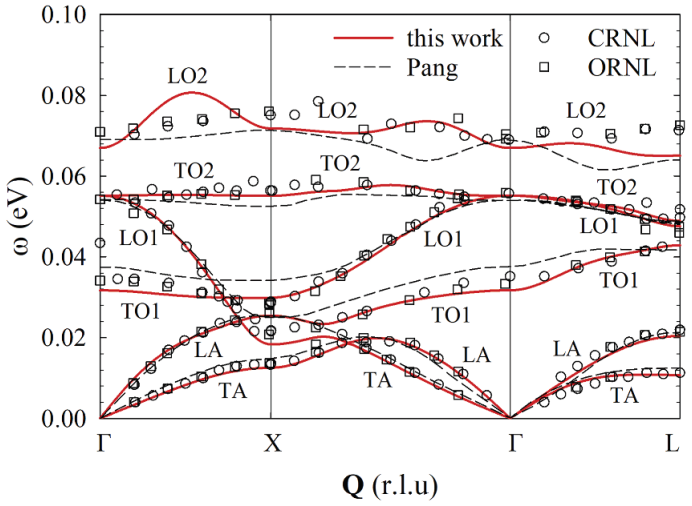


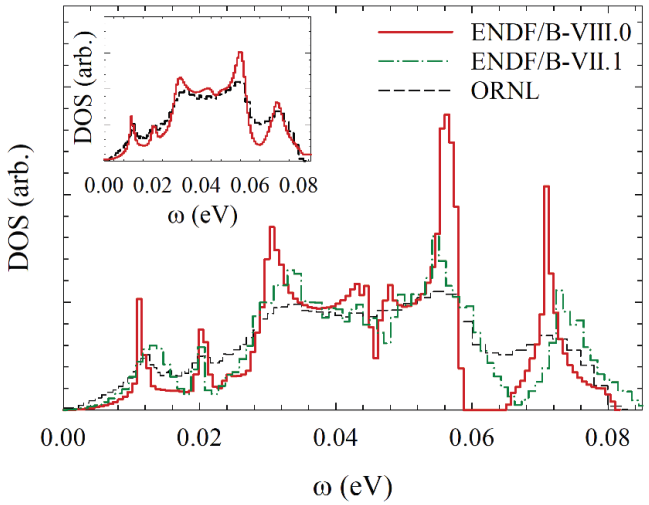
Uranium Dioxide

- VASP DFT Framework
  - GGA-PBE Pseudopotential
  - 4.0 eV Effective Hubbard Term
  - Magnetic Structure Captured with Spin-Orbit-Coupling
    - AFM polarizations in x, z -> paramagnetic
    - 2x2x2 supercell (64 atoms)



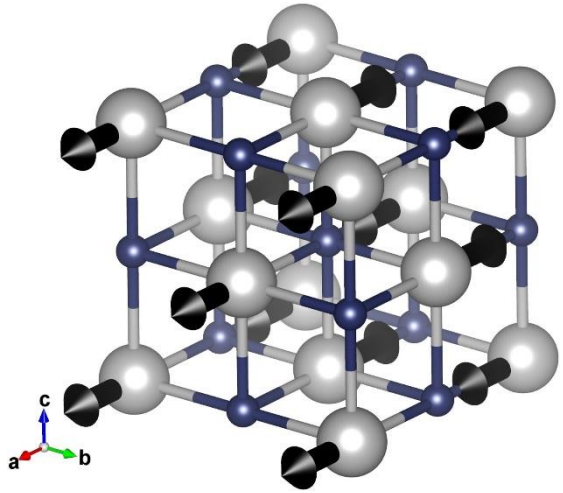


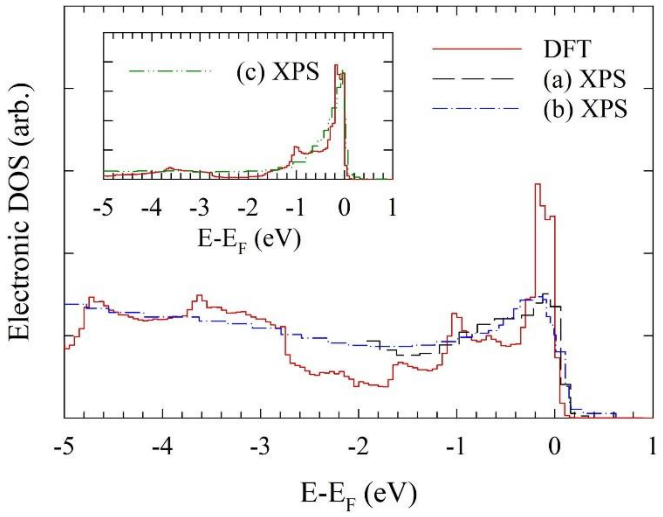


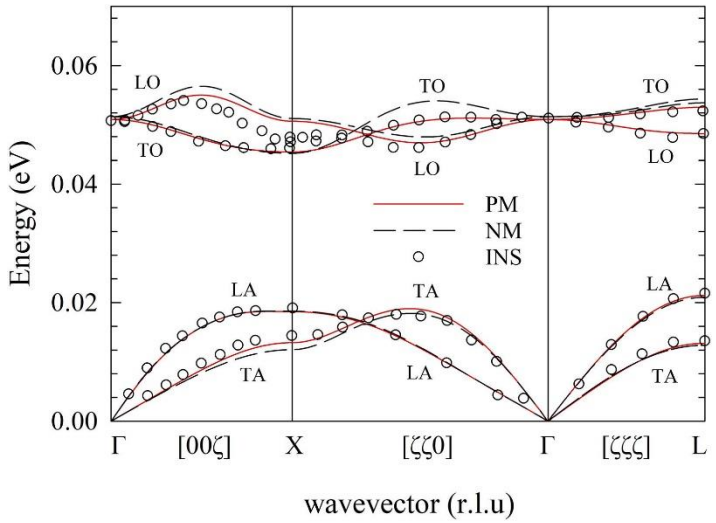


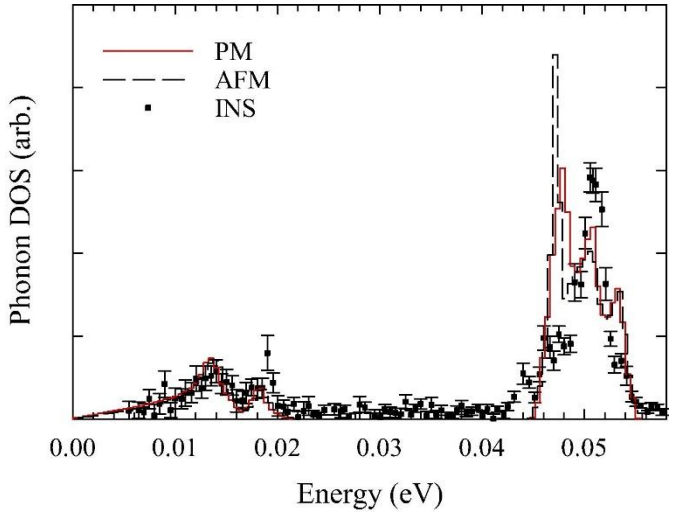
Uranium Nitride

- VASP DFT Framework
  - GGA-PBE Pseudopotential
  - No Hubbard Term
  - Magnetic Structure Captured with Spin-Orbit-Coupling
    - AFM polarizations in x, y, z -> paramagnetic
    - 2x2x2 supercell (64 atoms)



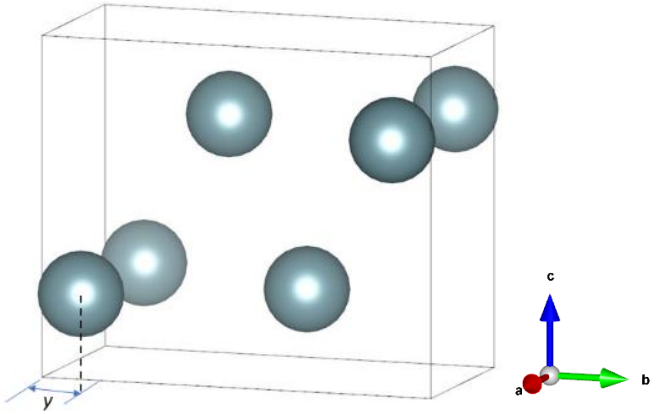




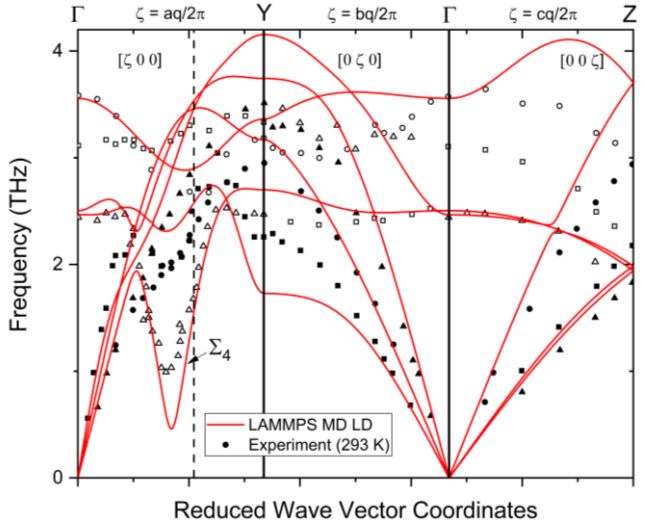


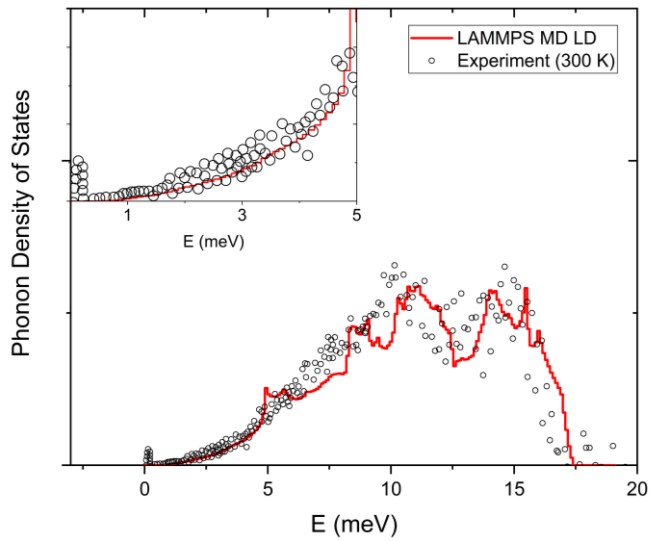
Uranium-Metal

- Molecular Dynamics Lattice Dynamics
  - Temperature dependence
  - Short times only
    - EAM potential
    - 20x10x10 supercell (20,000 atoms)
    - 0.04Å displacement



	B (GPa)	G (GPa)	σ (Å)
Experiment (50 K)	111	---	---
Experiment – 2	97.9	73.1	0.20
Experiment – 3	135.5	---	---
Experiment – 4	---	59-84	0.19-0.28
This Work (MD)	137	56	0.32



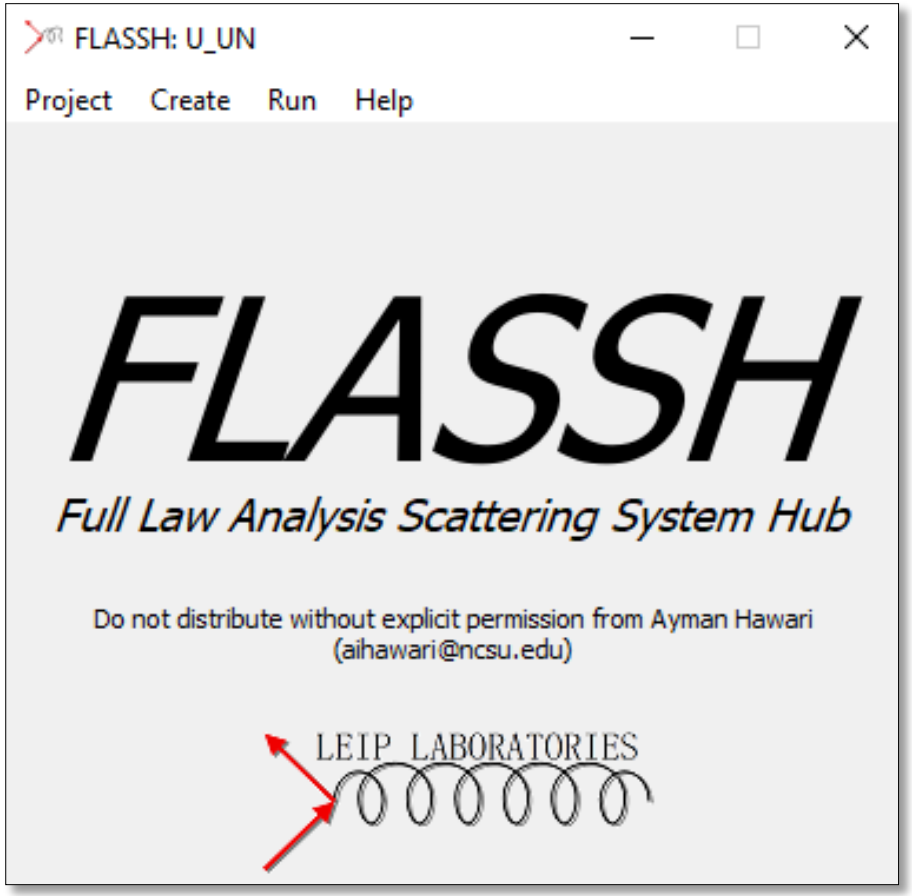


FLASSH

- ***FLASSH*: Full Law Analysis Scattering System Hub**
  - *M*odern thermal scattering evaluation code
  - Improves the physics of TSLs
  - Convenient user interface
  - Advanced physics

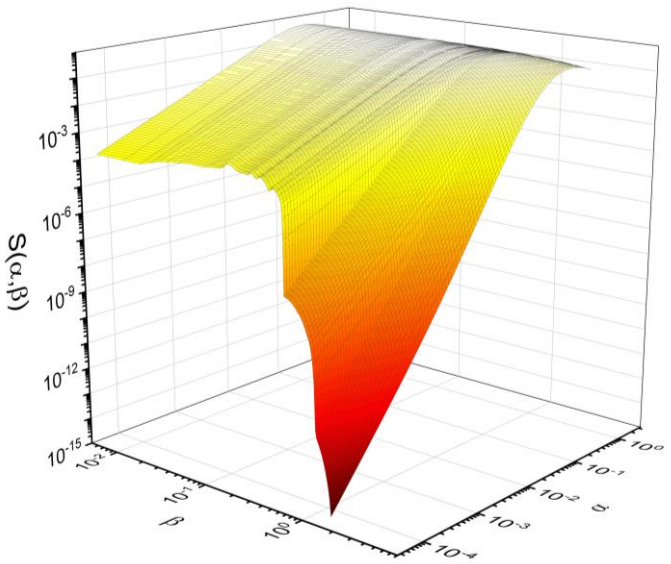
$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \frac{1}{4\pi}\sqrt{\frac{E'}{E}}\left[\sigma_{coh}S(\alpha,\beta) + \sigma_{inc}S_s(\alpha,\beta)\right]$$

$$S(\alpha,\beta) = \frac{1}{k_B T}\frac{1}{2\pi\hbar}\int e^{i(\vec{\kappa}\cdot\vec{r}-\omega t)}G(\vec{r},t)d\vec{r}dt$$



TSL Evaluations

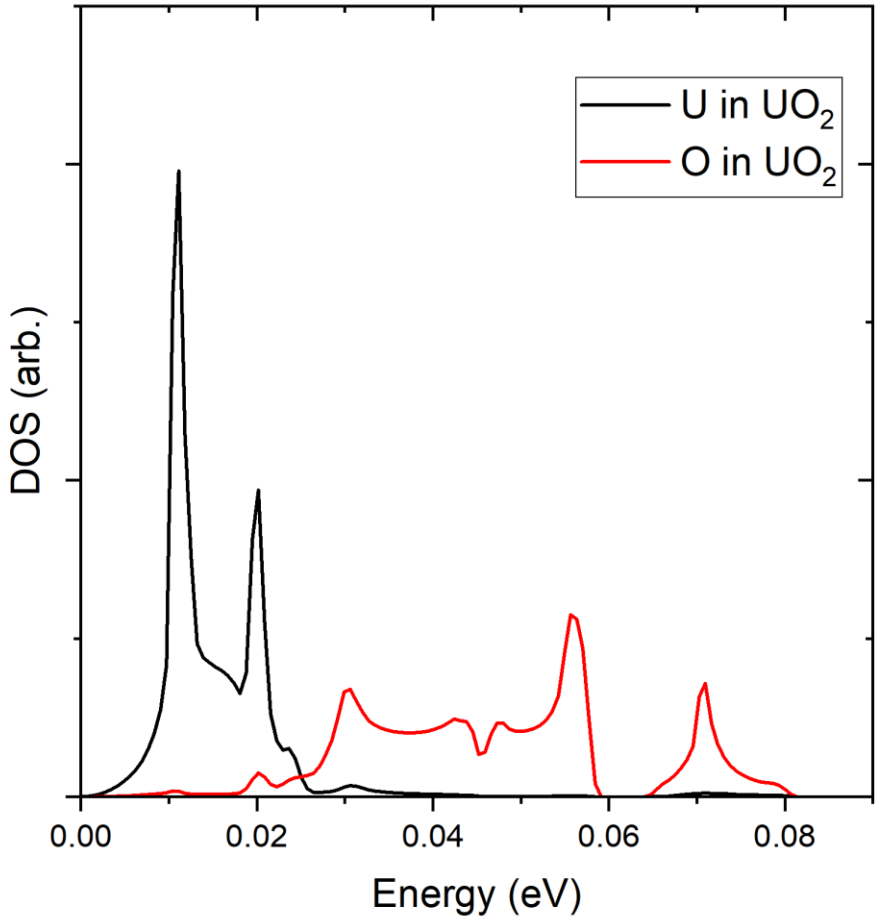
- **Updates to Existing Libraries**
  - Updated lattice parameters used to evaluate the coherent elastic
  - Updated input free atom cross sections and masses to reflect the current ENDF/B-VIII.0 values
  - Evaluations completed with *FLASSH*




```
 1.840000+2 2.330248+2          -1           0           0           0  84 1451
 0.000000+0 0.000000+0           0           0           0           6  84 1451
 1.000000+0 5.000000+0           0           0          12           8  84 1451
 0.000000+0 0.000000+0           0           0          31           3  84 1451
 U(UO2)     LEIP LAB    EVAL-SEP22 N.C. Fleming, A.I. Hawari             84 1451
                        DIST-                                            84 1451
----ENDF/B-VIII.0      MATERIAL  84                                      84 1451
-----THERMAL NEUTRON SCATTERING DATA                                     84 1451
------ENDF-6 FORMAT                                                     84 1451
                                                                         84 1451
  Temperatures = 296 400 500 600 700 800 1000 1200 K                     84 1451
                                                                         84 1451
 HISTORY                                                                 84 1451
 -------                                                                 84 1451
 This library was produced by the Low Energy Interaction Physics         84 1451
 (LEIP) group at NC State University, USA. The inelastic                 84 1451
 scattering thermal scattering law data for UO2 were developed           84 1451
 using ab intio lattice dynamics methods [1,2]. The Full Law             84 1451
 Analysis Scattering System Hub (FLASSH) code was used to                84 1451
 produce File 7 MT=2 and 4 for U in UO2 and O in UO2 [3]. MAT=84          84 1451
 and ZA=184 were used for U in UO2 (HEU).                                84 1451
                                                                         84 1451
 REFERENCES                                                              84 1451
 ----------                                                              84 1451
 1. A.I. Hawari, "Modern Techniques in Inelastic Thermal Neutron         84 1451
    Scattering Analysis," Nuclear Data Sheets 118 (2014) 172.            84 1451
                                                                         84 1451
 2. J.L. Wormald, A.I. Hawari, "Ab Initio Generation of Thermal          84 1451
    Scattering Law for Uranium Dioxide," Trans. Am. Nucl. Soc.,          84 1451
    115 (2016).                                                          84 1451
                                                                         84 1451
 3. N. C. Fleming et al., "FLASSH 1.0: Full Law Analysis                 84 1451
    Scattering System Hub," Trans. Am. Nucl. Soc., 125 (2021).           84 1451
                                                                         84 1451
```

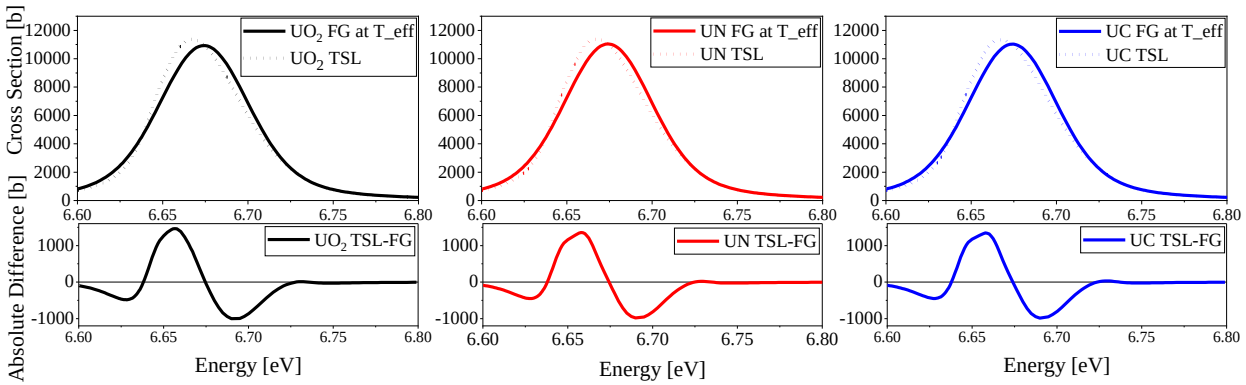
Enrichment Evaluations

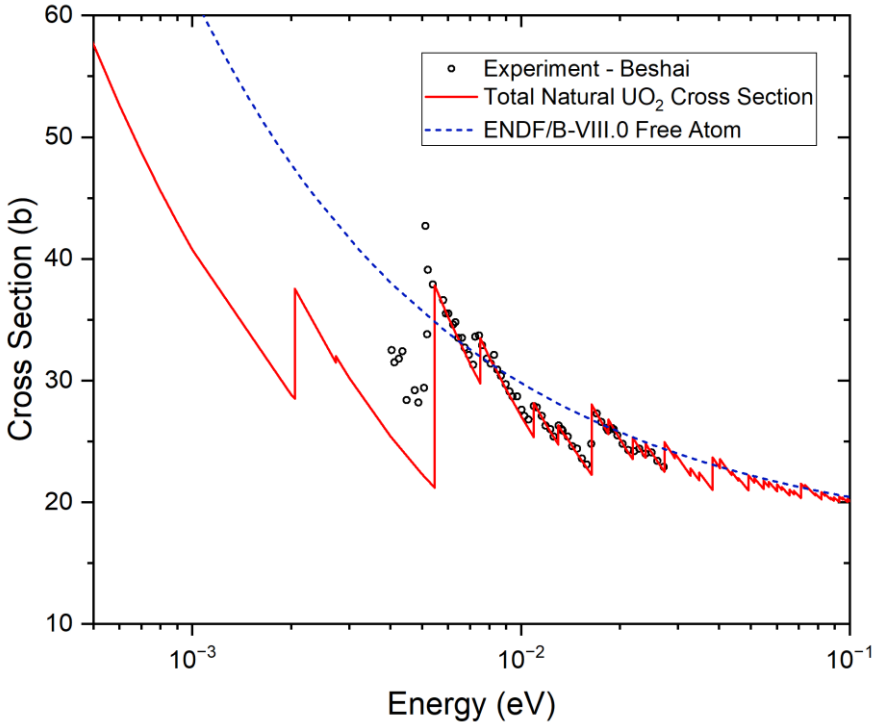
- TSL Evaluations for Varying Enrichment
  - Inputs Varied
    - **Mass**
    - **Free Atom Cross Section**
  - DOS constant
  - Natural (NIST natural elemental isotopic weighting)
  - 5% U-235
  - 10% U-235
  - HEU (100% U-235)

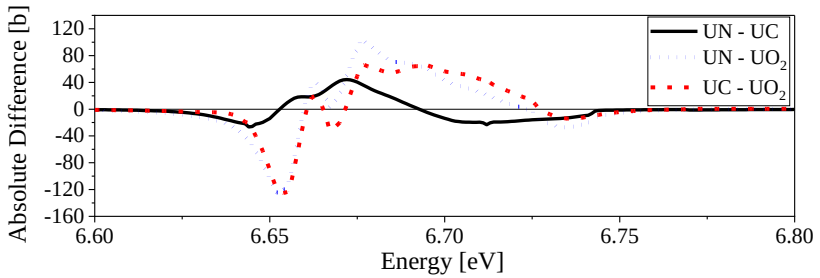


Uranium Cross Sections

- **Benchmarks**
  - Total Cross Section Measurements
  - Doppler Broadened Resonances
  - Natural Cross Sections

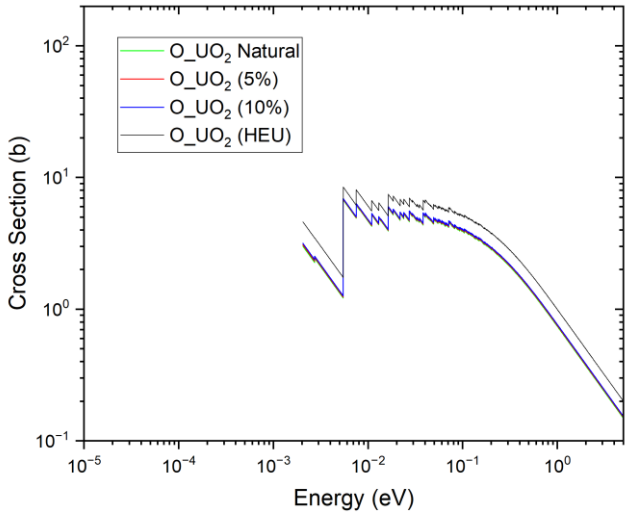


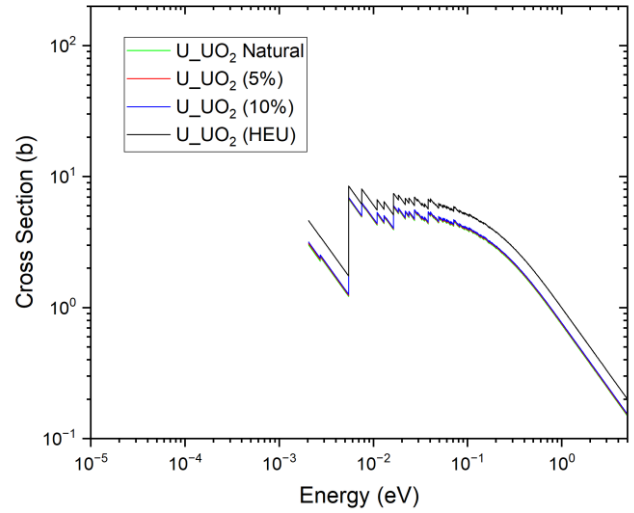


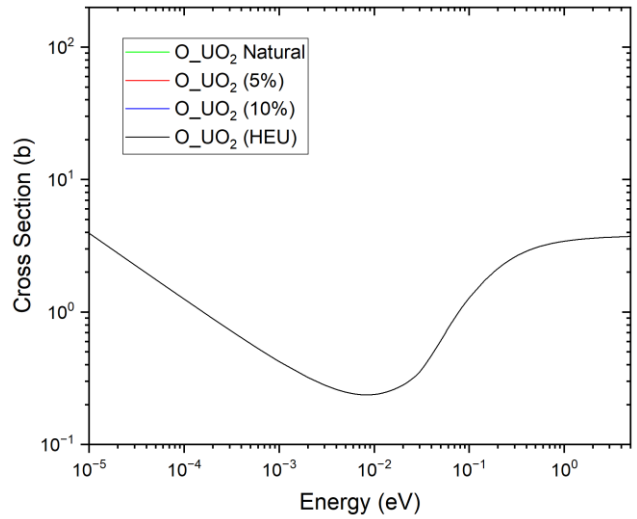


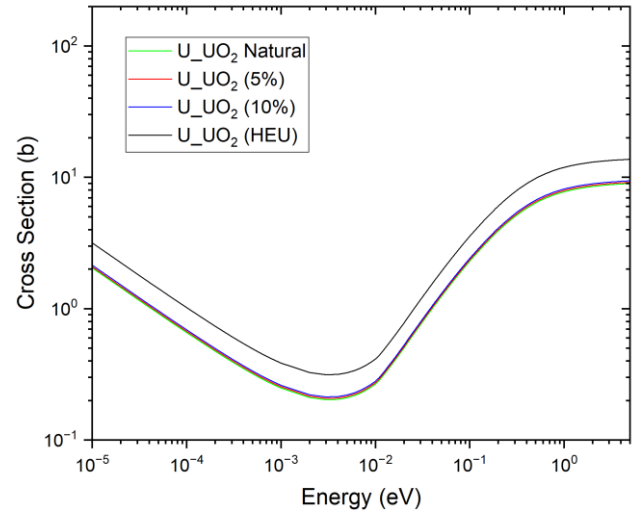
Uranium Dioxide

- **UO_2 TSLs**
  - Coherent elastic reflection of compound demonstrates effects from the varies cross section and mass impacts of the uranium weighting
  - Inelastic cross sections are a reflection of the unchanged DOS



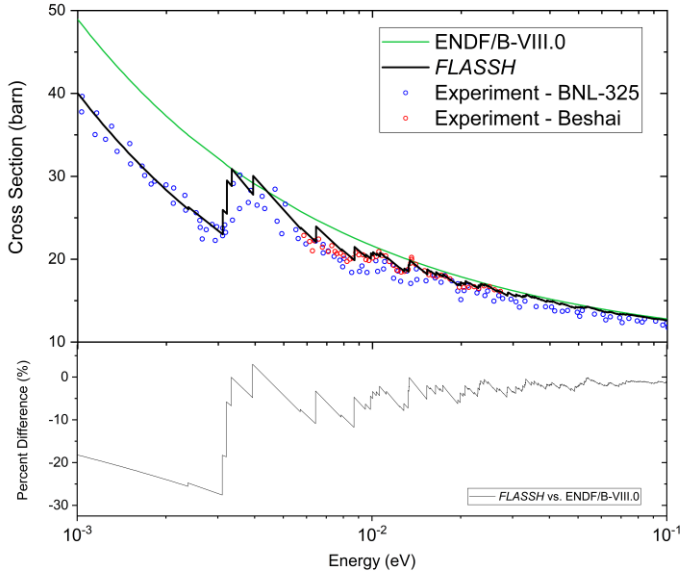


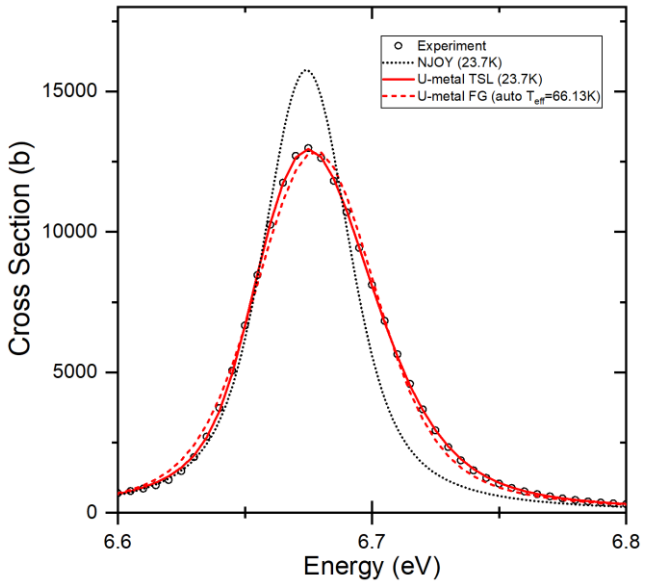


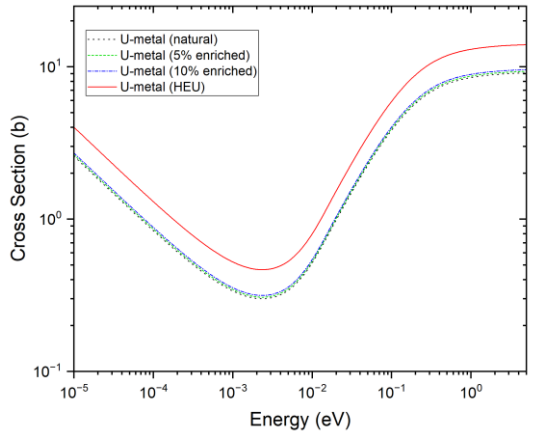


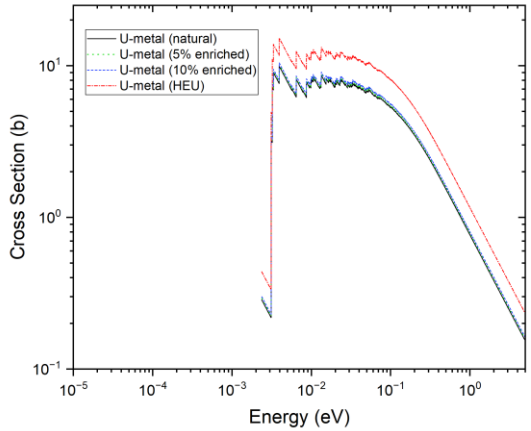
Uranium-Metal

- **U-metal TSLs**
  - Benchmarked against total cross section measurements
  - Demonstrated accurate structure in ability to capture the correct structure of U-metal Doppler broadened resonance structure
  - Enrichment-dependent libraries available



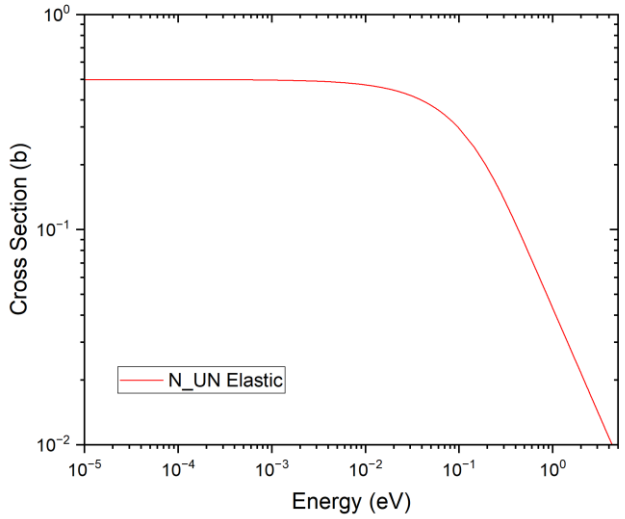


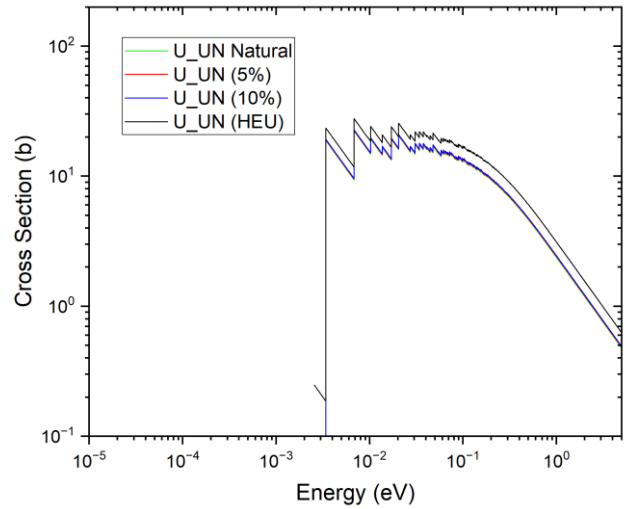


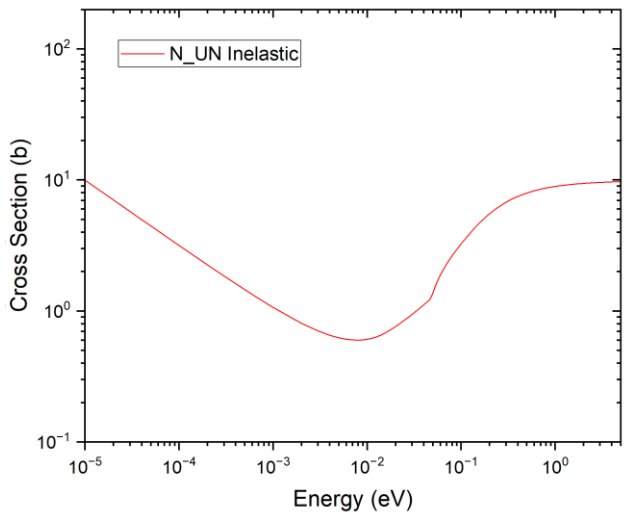


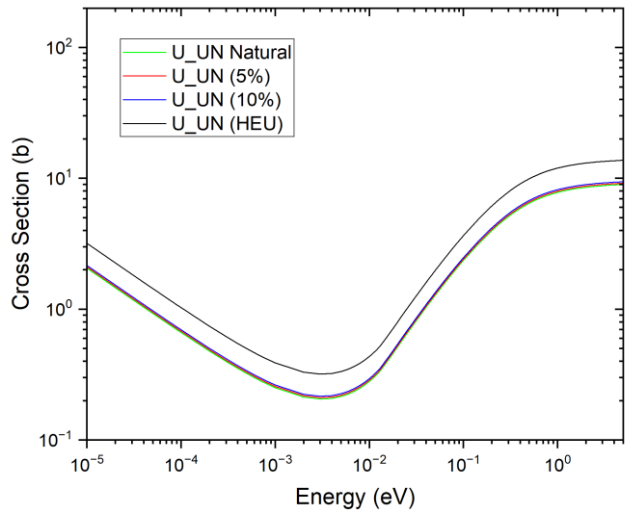
Uranium Nitride

- **UN TSLs**
  - Coherent elastic stored with uranium file
  - Incoherent elastic stored with nitrogen
  - Inelastic cross sections are a reflection of the unchanged DOS



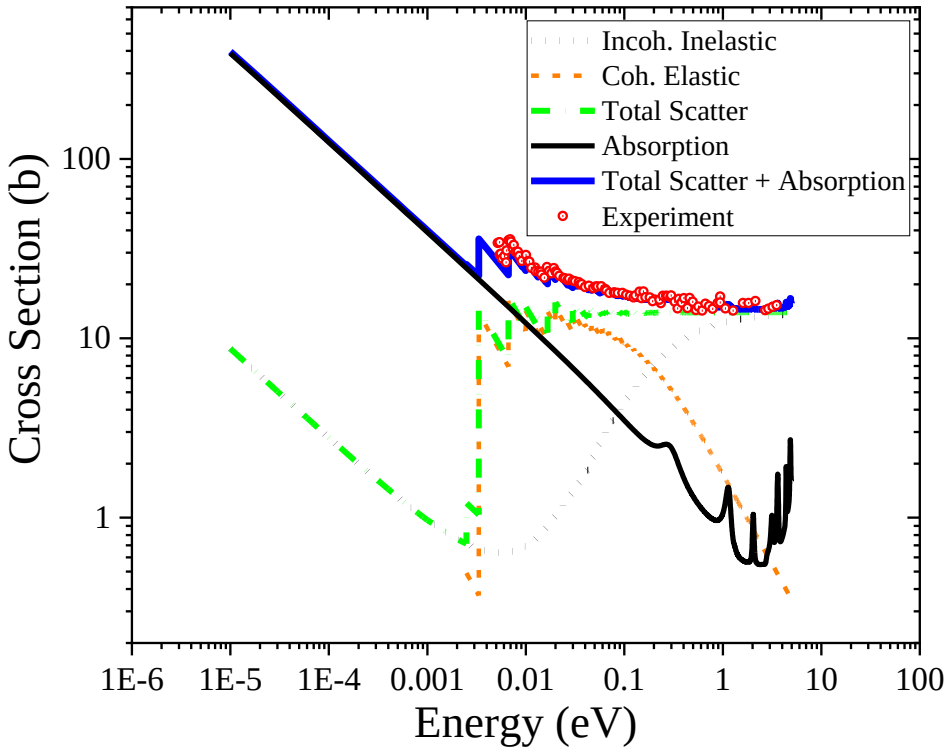


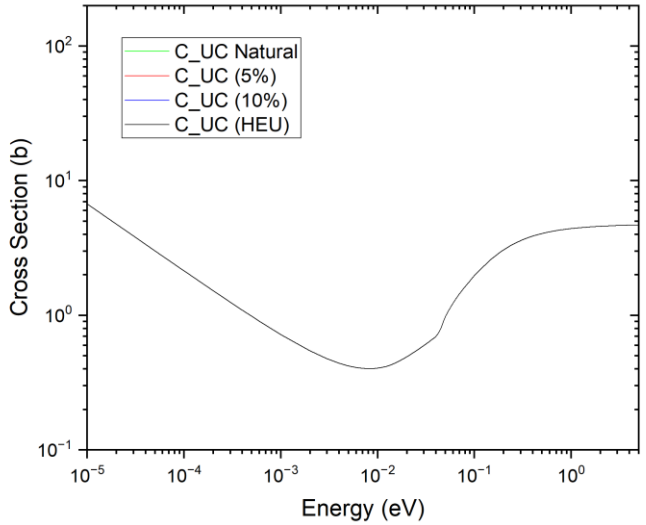


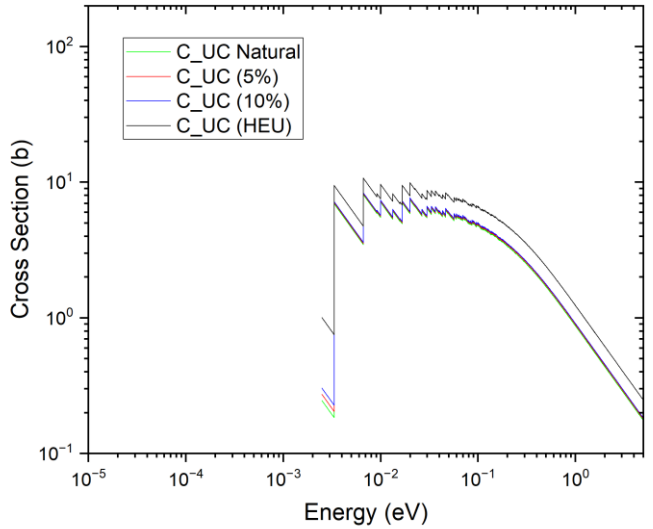


Uranium Carbide

- **UC TSLs**
  - Benchmarked against total cross section measurements
  - Enrichment-dependent libraries available
    - Carbon and Uranium Libraries







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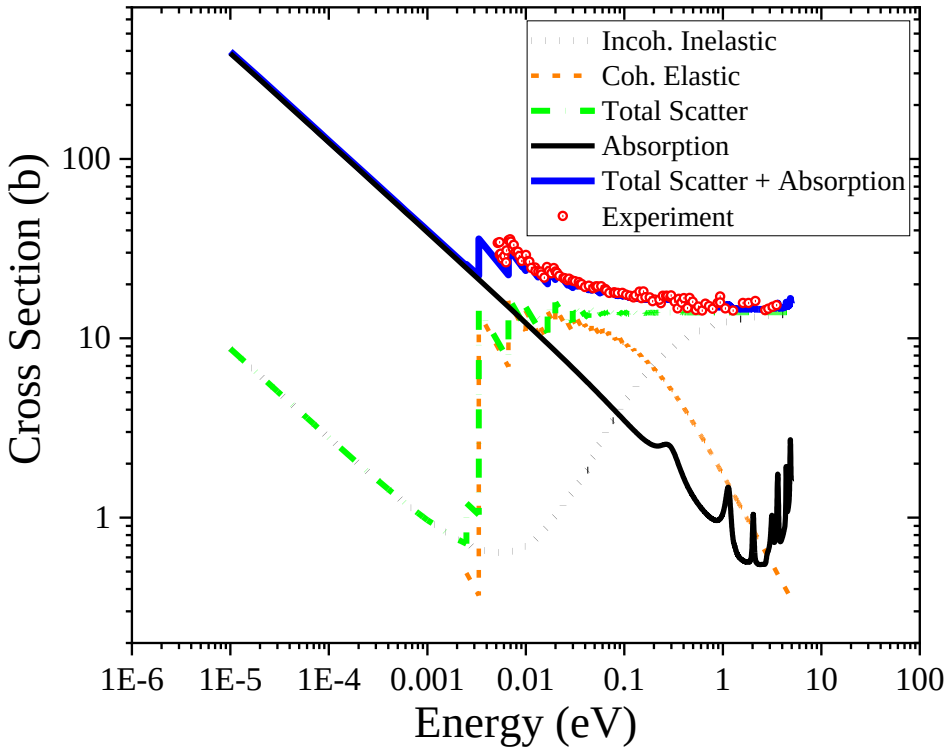
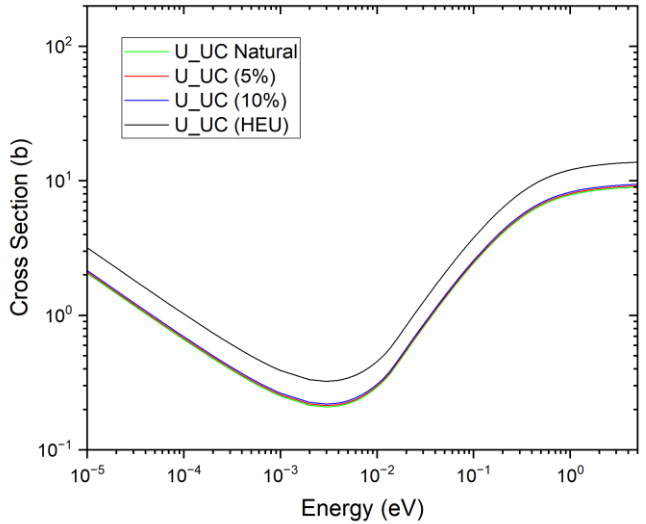
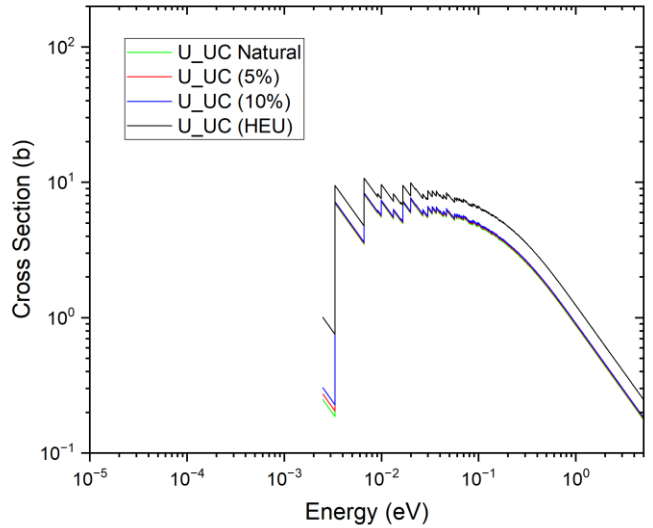
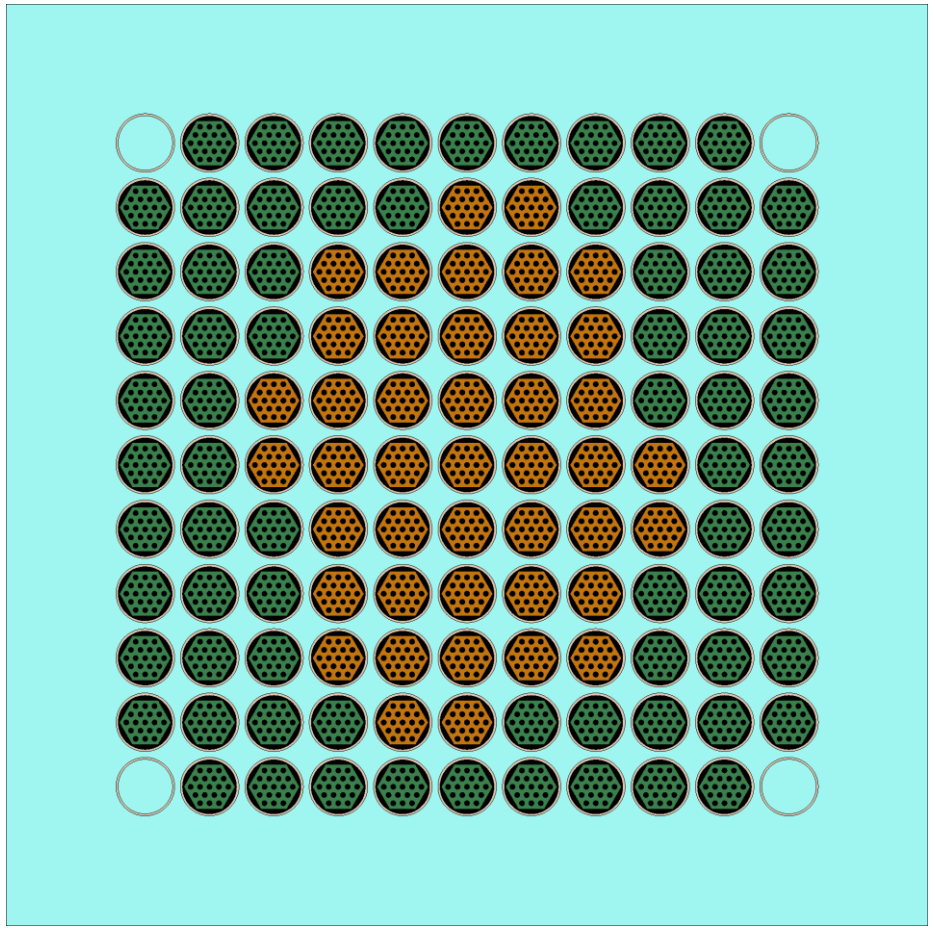






Benchmark Applications

- **HEU-COMP-THERM-002**
  - Uranium carbide fuel matrix (93.15% U-235 enriched)
  - Water and polyethylene moderators
  - Room temperature
  - Thermal energy spectrum
  - Other TSLs:
    - Light water
    - Polyethylene



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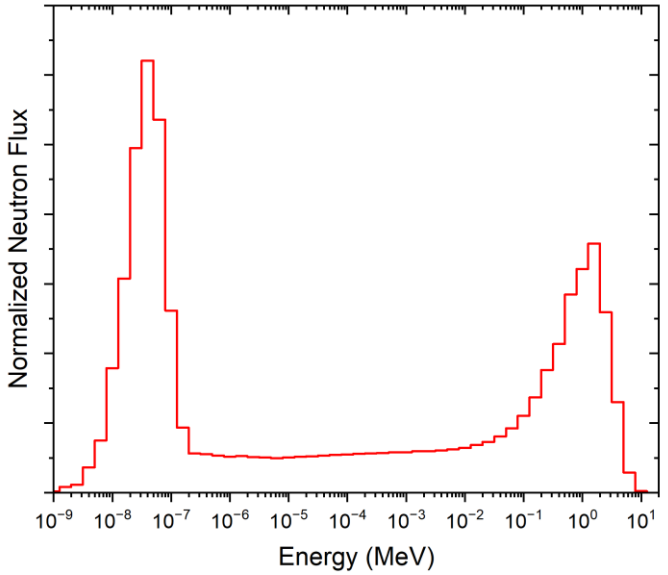

Preliminary	k_{eff}
Benchmark k_{eff}	1.0011 ± 0.0069
ENDF/B-VIII.0	1.01335 ± 0.0004
ENDF/B-VIII.0 + Natural UC TSL	1.01023 ± 0.0004
ENDF/B-VIII.0 + HEU UC TSL	1.00848 ± 0.0004
Impact from HEU TSL (pcm)	-487

NC STATE UNIVERSITY

Summary

New and updated uranium fuel evaluations have been submitted to the ENDF/B libraries. These include vital fuel materials U-metal, UC, UN, and UO_2.

- **Enrichment-Dependent Evaluations –** directly correlates to experimental data or benchmark for comparison
- **Improved Inputs –** corresponds with experimental structure and ENDF/B-VIII.0 accepted values for cross section and mass
- **QA Internal Checks Complete –** submitted to ENDF/B after passing through formal internal quality assurance checks

LEIP LABORATORIES

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Thank You