NAVAL NUCLEAR LABORATORY

Update on ENDF/B-VIII.1 TSLs for Moderator and Fuel Materials

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Objective

- Provide status update on TSLs for moderator and fuel materials available in ENDF/B-VIII.1
- Focus on materials relevant to HALEU deployment and Advanced Reactor design
  - TSLs for many materials already developed
- Discuss need for well characterized benchmarks to drive improvements

ENDF/B-VIII.1 TSL Updates

- Renaissance in TSL Evaluation Methods
- 114 evaluations for 69 materials in Thermal Neutron Scattering (File 7) sublibrary
  - Fuel, moderators, and special purpose (cold neutrons/filters)
  - 23 material re-evaluations; 32 new material evaluations
  - New MAT numbers
- New physics or material conditions (select evaluations)
  - Mixed elastic scattering
  - Random alloy theory
  - Coherent inelastic scattering (+Sd)
  - Multiple phases
  - ^{235}U enrichments (natural, 5%, 10%, HALEU, HEU, 100%)

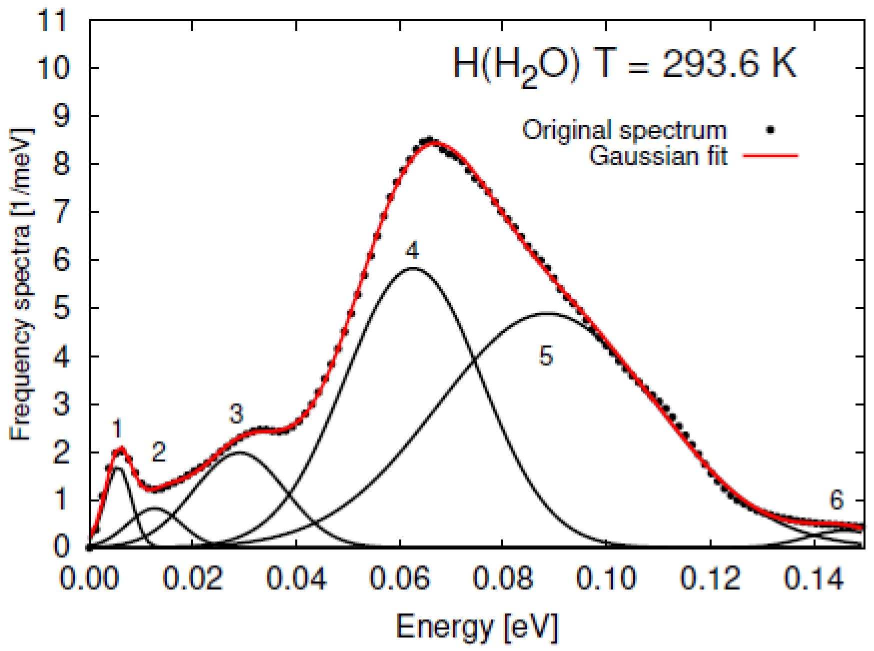
- Modern Evaluation Methodologies
  - Most evaluations are *ab initio* Lattice Dynamics (AILD) based
  - *ab initio* Molecular Dynamics (AIMD) beginning to be used
  - Experimentally adjusted AILD (exp+AILD) methods
- Evaluation codes
  - New *FLASSH* code generated 44 material evaluations (NNL and NCSU)
  - NJOY/LEAPR & NJOY+Ncrystal (ESS, ORNL)
- ENDF/B-VIII.1 released August 30, 2024

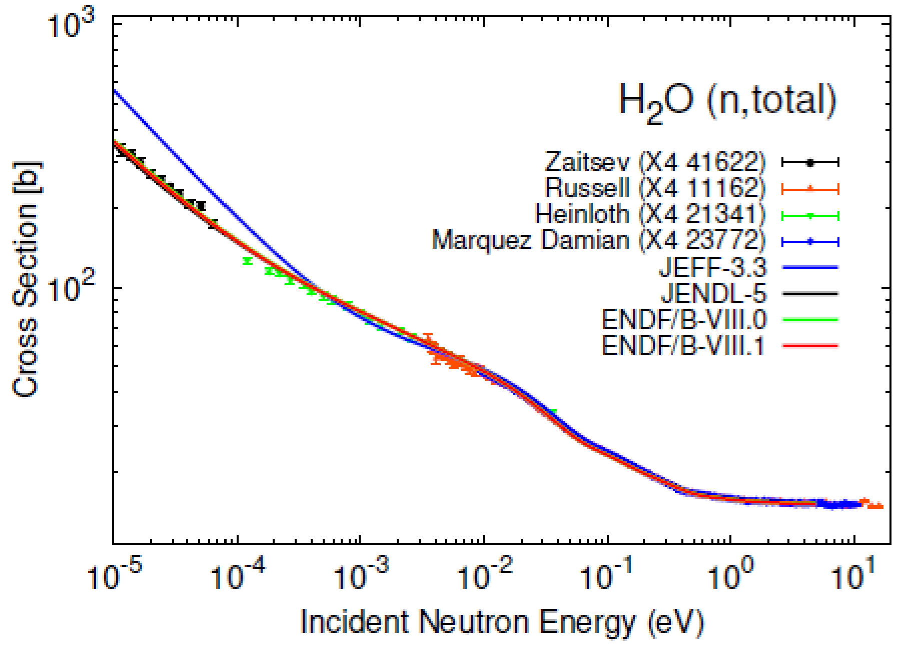
Advanced Reactor Coolants

Material	Evaluator	Atomistic Method	New Physics	New Condition	Status
H_2O	CAB/ESS	MD+interpolation	Diffusion model	More Temps, Lower Temps	Reevaluation
D_2O	CAB	MD			ENDF/B-VIII.0
FLiBe	NCSU	MD			New

H_2O

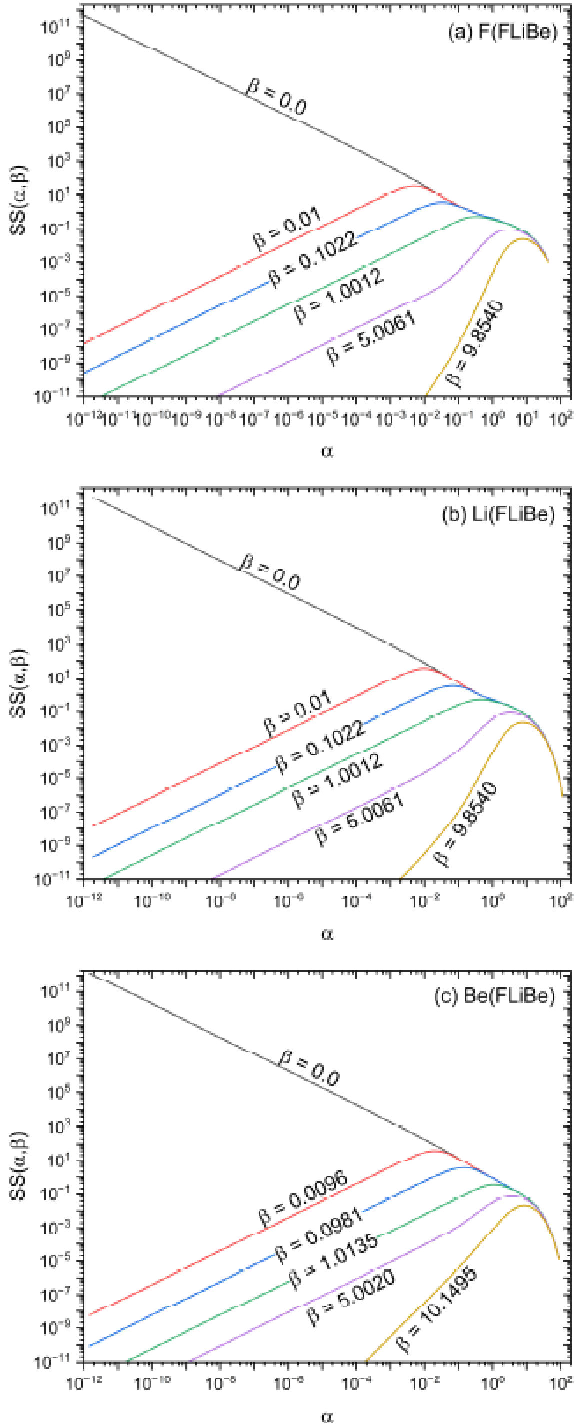
- Evaluation with NJOY + Gaussian PDOS fit
  - ΔT=5 K for 273.15 – 647.1 K
  - ΔT=50 K for 650 – 1000 K
- Same fundamental physical model used in ENDF/B-VIII.0 H(H2O)
- Reevaluation
  - Liquid, MT4 only
  - Temperature-dependent analytic material model fit to MD and exp (diffusion)
  - Retains assumption of constant material properties for critical phase above 647.1 K

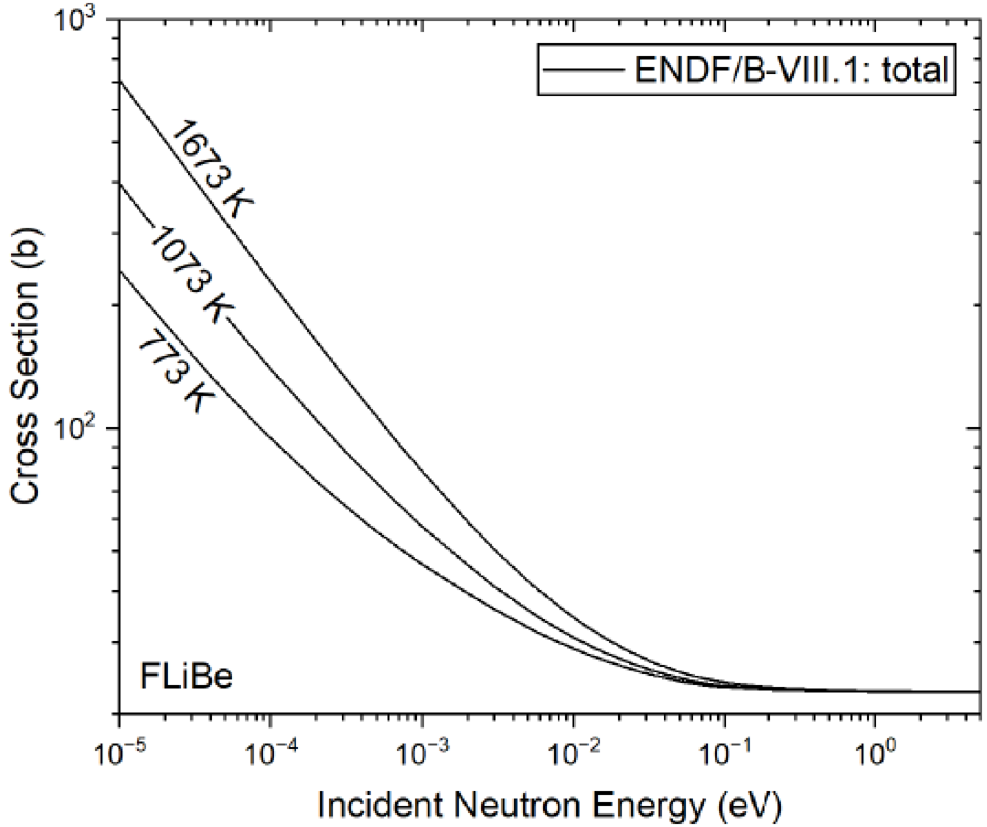




FLiBe

- Evaluations with *FLASSH* + MD
  - 773, 873, 923, 973, 1073, 1173, 1273, 1473, 1673 K
- New evaluation
  - F(FLiBe)
  - ^{7}Li(FLiBe)
  - Be(FLiBe)
  - Liquid, MT4 only



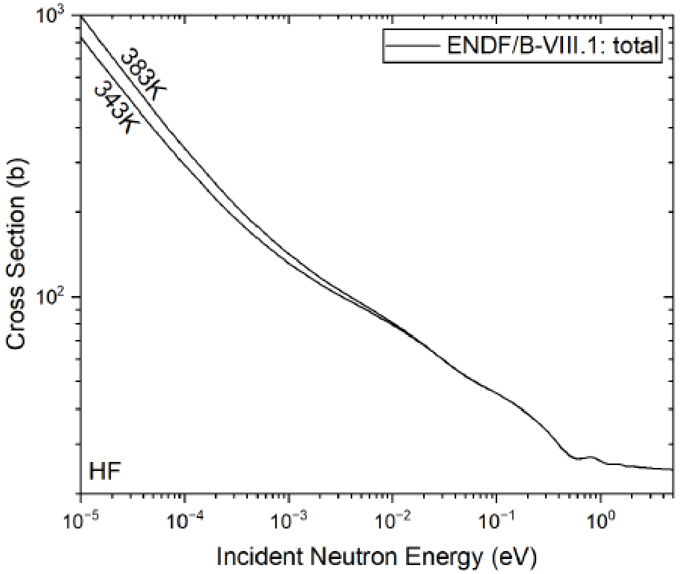


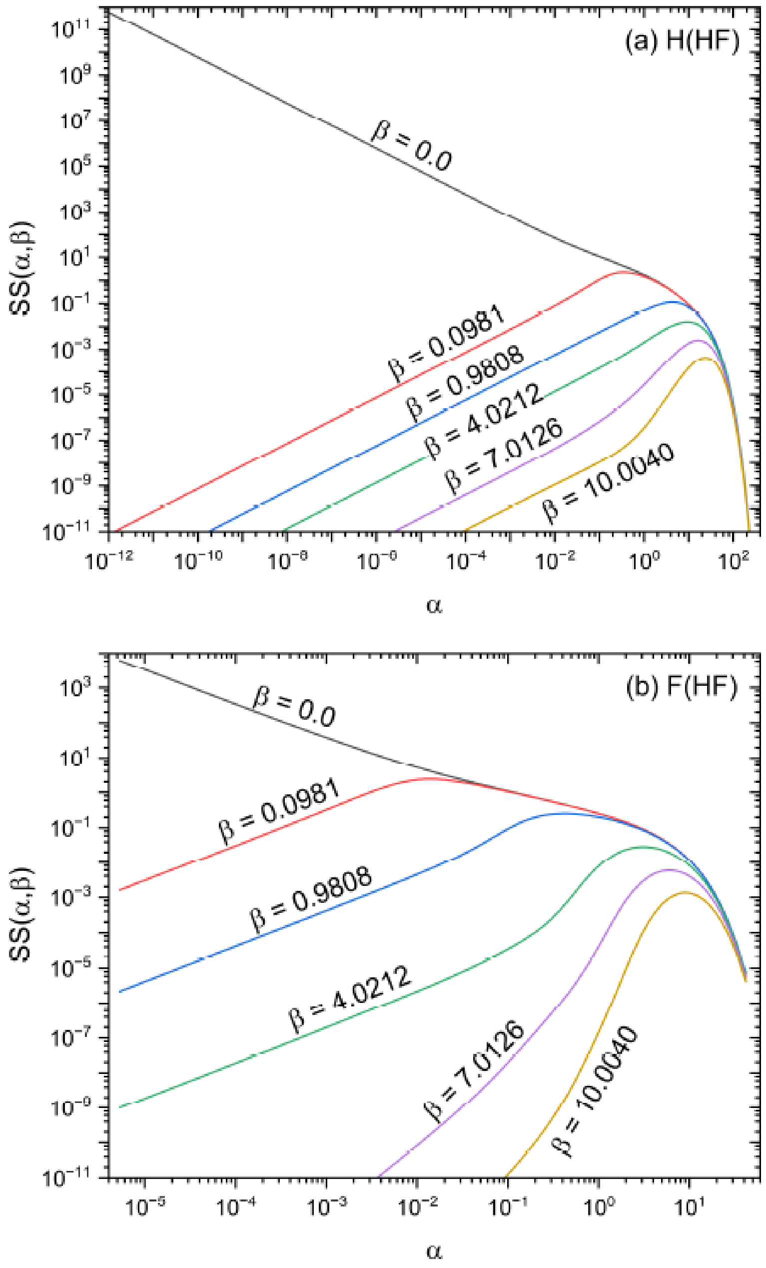
Facility and Transportation NCS

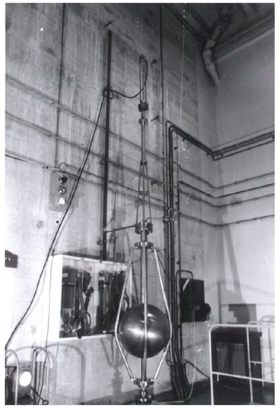
Material	Evaluator	Atomistic Method	New Physics	New Condition	Status
HF	NCSU	MD			New
Heavy Paraffinic Oil	NCSU	MD			New
Polyethylene	NCSU	MD			ENDF/B-VIII.0
Hexagonal Ice	NNL	AILD			ENDF/B-VIII.0

Anhydrous HF

- Evaluations with *FLASSH* + MD
  - 343, 348, 353, 363, 373, 383 K
- New Evaluation
  - H(HF) and F(HF)
  - Liquid, MT4 only
  - ^{19}F pointwise evaluation
- Modeling HF contamination in UF_6 cylinders







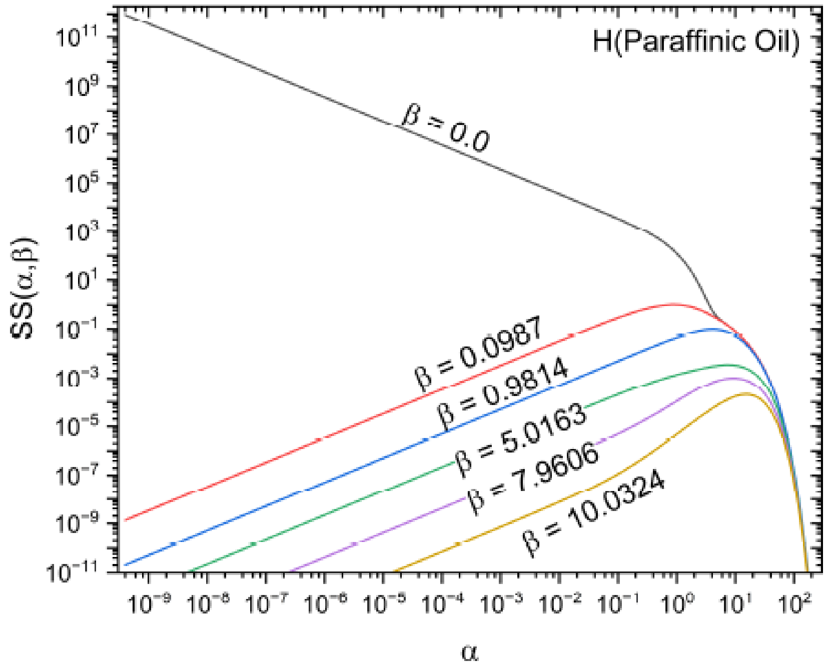
Case	Benchmark 1	ENDF/B-VIII.0 No HF TSL 2	C-E (pcm) (2-1)	ENDF/B-VIII.1 ^{19}F No HF TSL 3	C-E (pcm) (3-1)	ENDF/B-VIII.1 ^{19}F HF TSL 4	C-E (pcm) (4-1)
1	1.0000	1.03604	3604	1.02298	2298	1.01614	1614
2	1.0000	1.02641	2641	1.01417	1417	1.00344	344
3	1.0012	1.02466	2346	1.01217	1097	0.99967	-153
4	1.0018	1.02899	2719	1.01582	1402	1.00231	51
5	1.0018	1.04124	3944	1.02719	2539	1.01225	1045
6	1.0025	1.02592	2342	1.01116	866	0.99702	-548

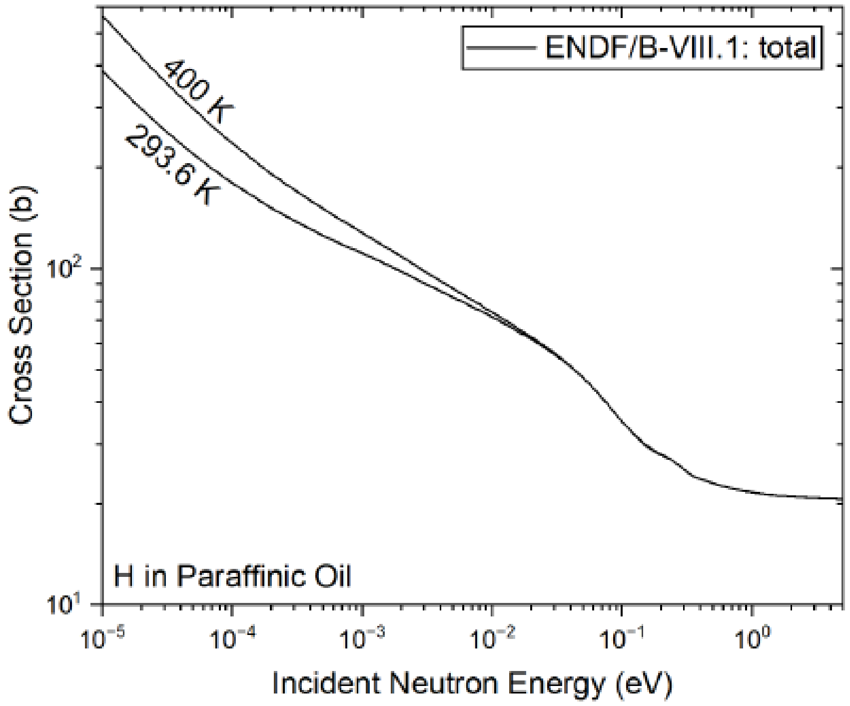
HEU-SOL-THERM-039
(HF)

- **Combination of ENDF/B-VIII.1 ^{19}F + HF TSL yielded significant improvement**
- **More work to be done on ^{19}F**

Heavy Paraffinic Oil

- Evaluations with *FLASSH* + MD
  - 293.6, 300, 325, 350, 375, 400 K
- New evaluation
  - H(Paraffinic Oil)
  - Liquid, MT4 only
- Intended for use in modeling machining oils



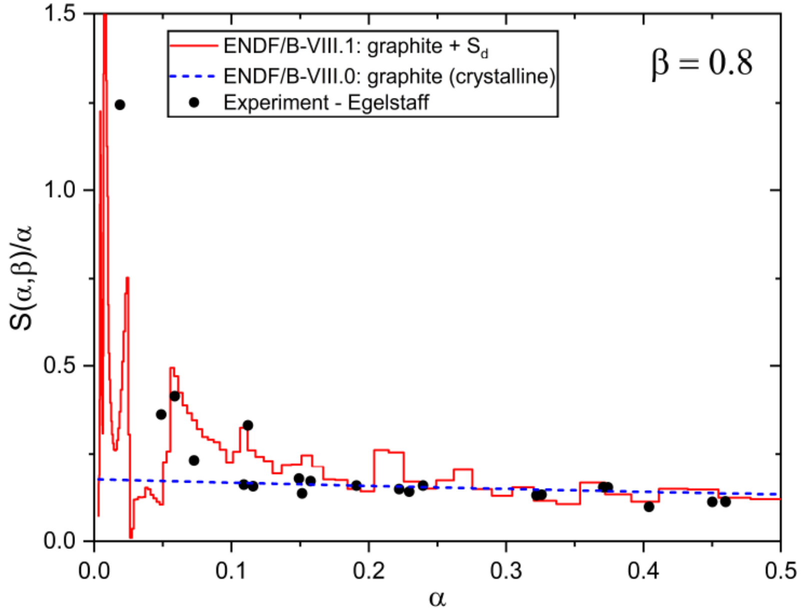


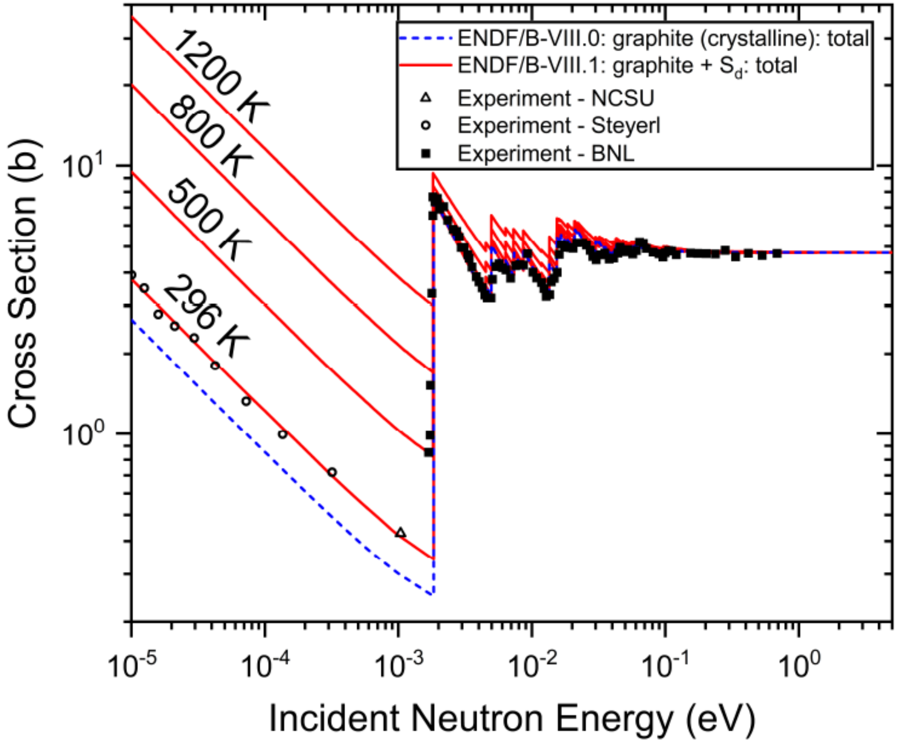
Graphite + SiC

Material	Evaluator	Atomistic Method	New Physics	New Condition	Status
Crystalline Graphite	NCSU	AILD	Sd, Exp. Lat. Param.		Reevaluation
Reactor Graphite (10%, 20%, 30% porosity)	NCSU	MD	Porosity (random)	20% porous	ENDF/B-VIII.0, New
SiC	NCSU	AILD	Exp. Lat. Param.		Reevaluation

Crystalline Graphite

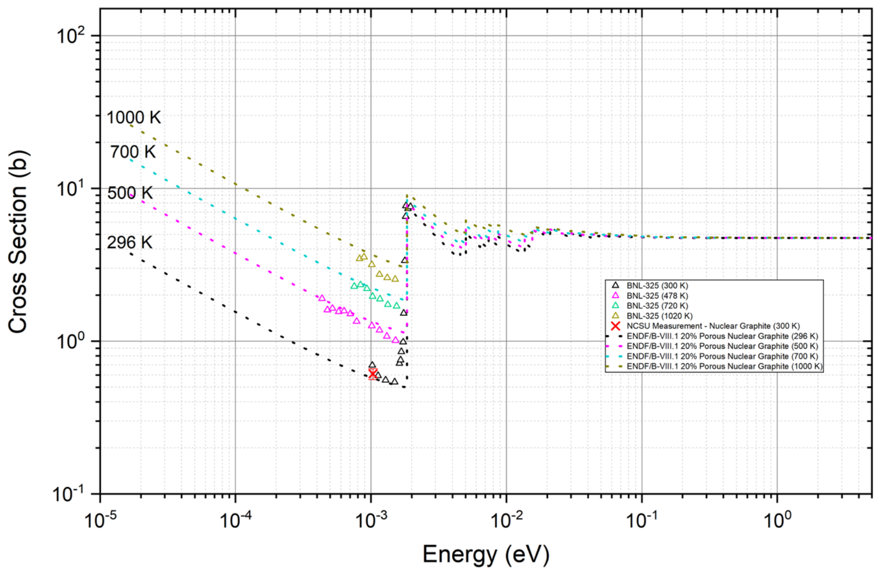
- Evaluations with *FLASSH* + AILD
  - 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000 K
- Two Evaluations
  - Crystalline Graphite
  - Crystalline Graphite+S_d (distinct effects)
  - MT2 now uses exp lattice parameters
  - MT4 includes coherent inelastic in +S_d TSLs
    - Same as ENDF/B-VIII.0 model otherwise
  - Crystalline Graphite+Sd has improved agreement with historical measurements in sub-Bragg cutoff region

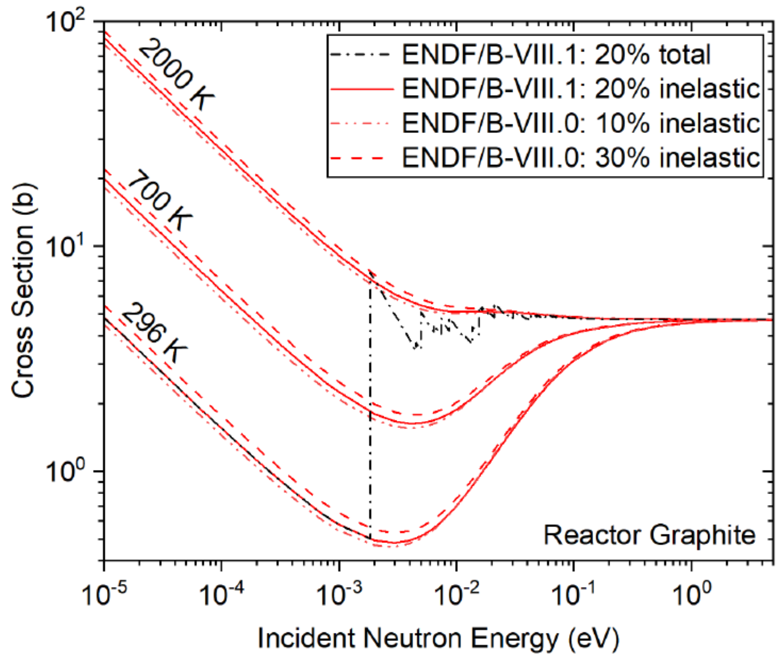




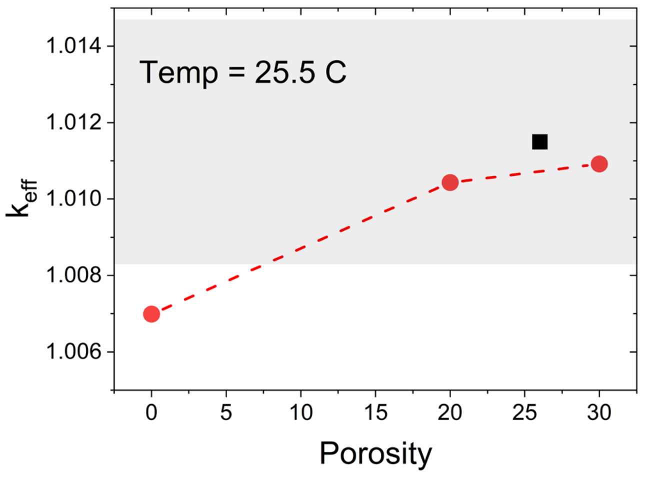
Reactor Graphite

- Evaluations with *FLASSH* + MD
  - 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000 K
- ENDF/B-VIII.0 included 10% and 30% porosity
- ENDF/B-VIII.1 adds 20% porosity
  - Same MD model as ENDF/B-VIII.0
- Random porosity model resolved historical discrepancy in sub-Bragg cutoff region with BNL-325 measurements on reactor graphite
- 30% porosity TSL performs better than crystalline graphite TSLs in new FUND-ORELA-ACC-GRAPH-PNSDT-001 benchmark in ICSBEP Handbook
- **Additional well characterized benchmarks sensitive to reactor grade graphite are needed**





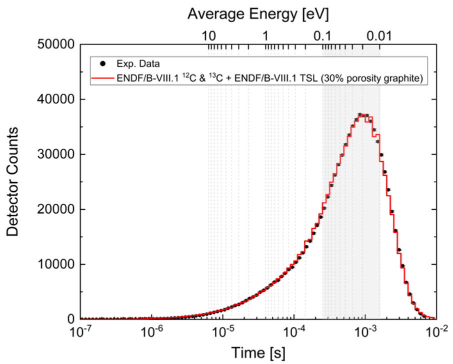
Reactor Graphite Validation



Density = 1.67 g/cm^3
Porosity ≈ 30%

VHTRC-GCR-EXP-001

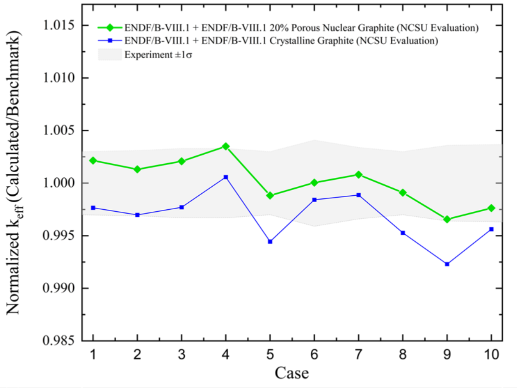
$$\text{Porosity}(\%) = \left(1 - \frac{\rho_{component}}{\rho_{ideal}}\right) \times 100\%$$



Cross Sections	Mean Absolute Deviation (%)
ENDF/B-VIII.0 + Cry	4.14%
ENDF/B-VIII.1 + Cry	4.09%
ENDF/B-VIII.1+S_d	5.01%
ENDF/B-VIII.1+30%	1.68%

Density = 1.66 g/cm^3
Porosity ≈ 30%

FUND-ORELA-ACC-GRAPH-PNSDT-001
(Nuclear Graphite)



Case	C-E (pcm)	
	Crystalline	20% Nuclear
1	235	204
2	303	137
3	230	188
4	57	322
5	707	146
6	258	12
7	83	91
8	344	95
9	782	385
10	529	247

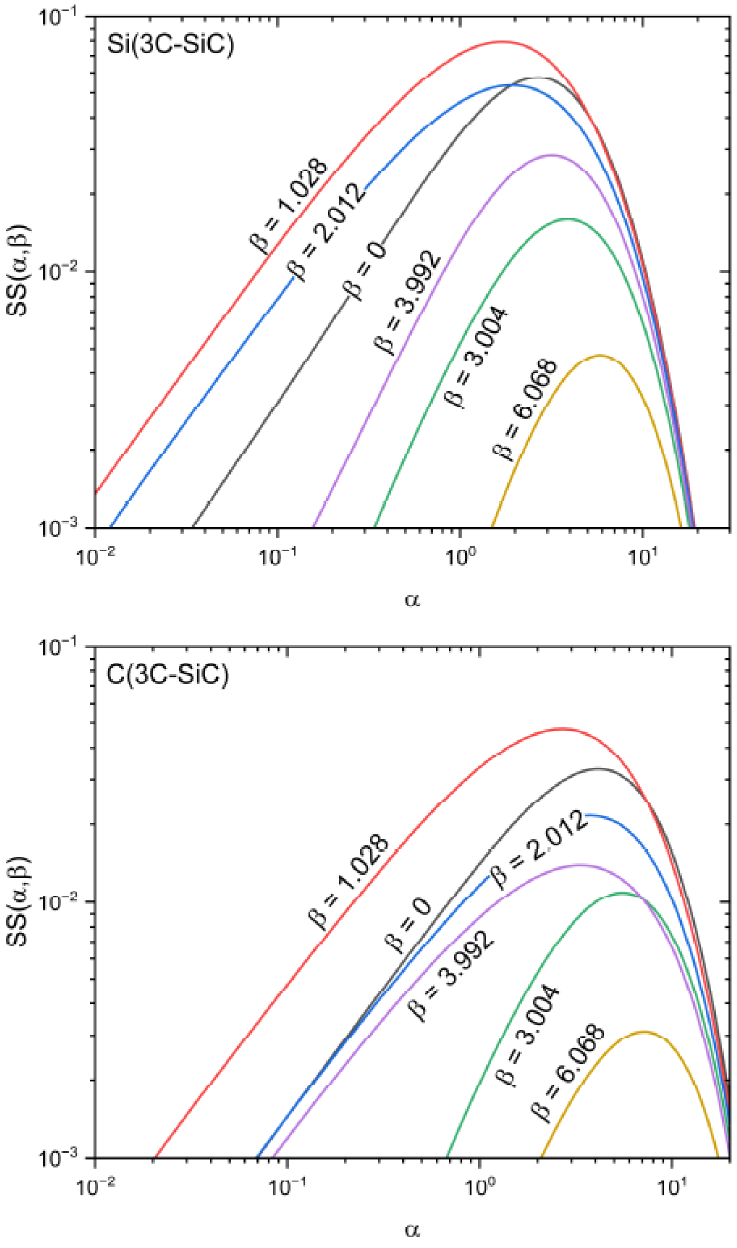
Density = 1.7 g/cm^3
Porosity ≈ 20-30%

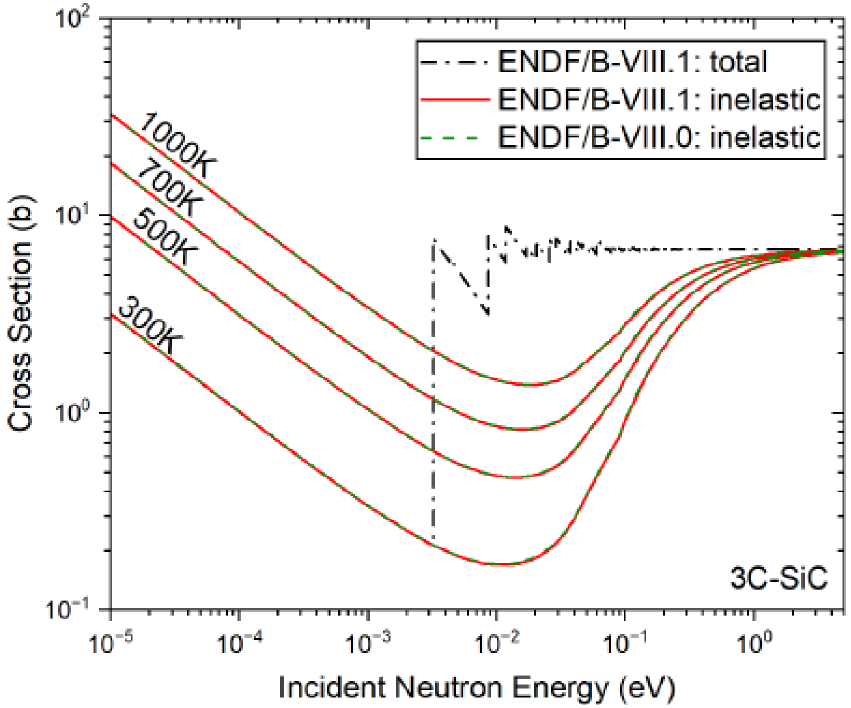
PROTEUS-GCR-EXP-001 to -004
(Nuclear Graphite)

From Ayman Hawari's Graphite History Presentation at 2024 NCSP TRP

SiC

- Evaluations with *FLASSH* + AILD
  - 296, 400, 500, 600, 700, 800, 1000, 1200 K
- Reevaluation
  - Si(SiC) and C(SiC)
  - Nuclide data changed from ^{28}Si and ^{12}C to natural Si and C
  - MT2 changes due to use of exp lattice parameter
  - MT4 same model as ENDF/B-VIII.0



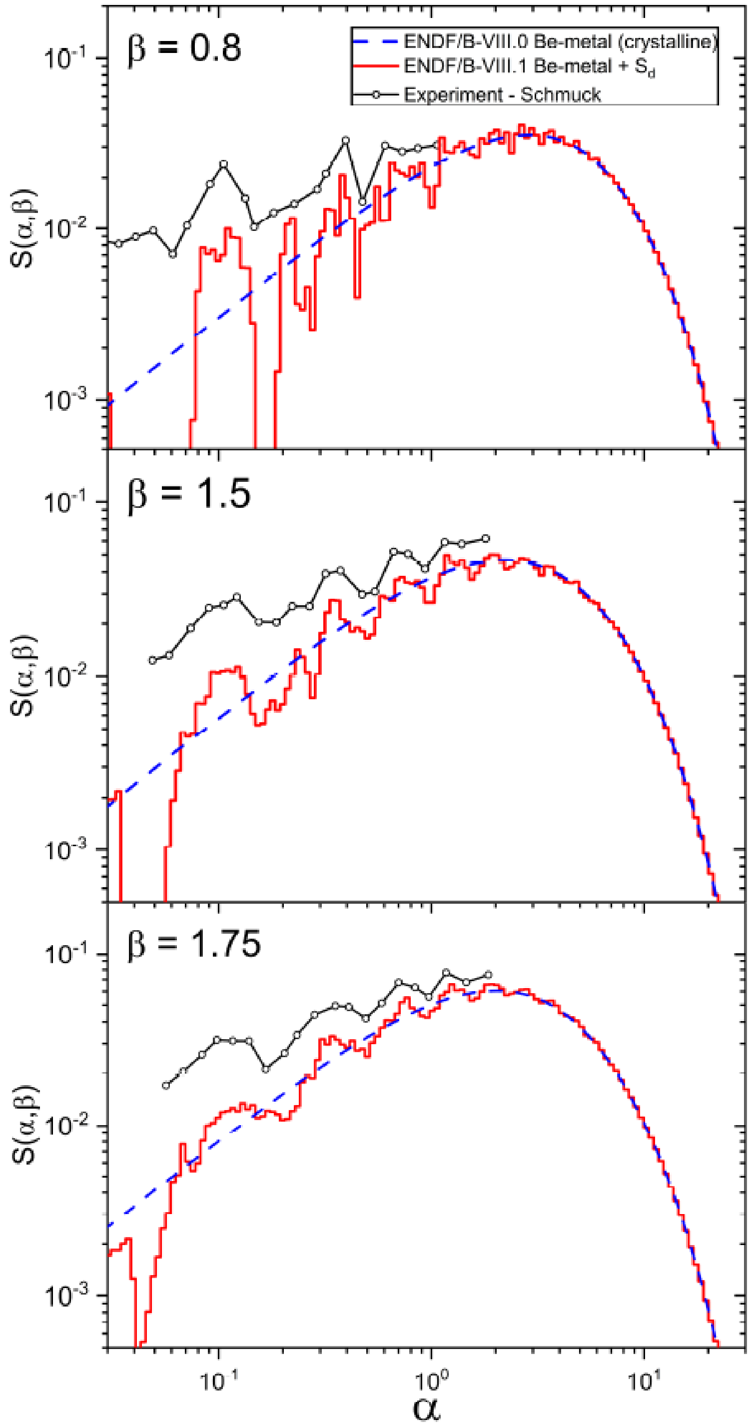


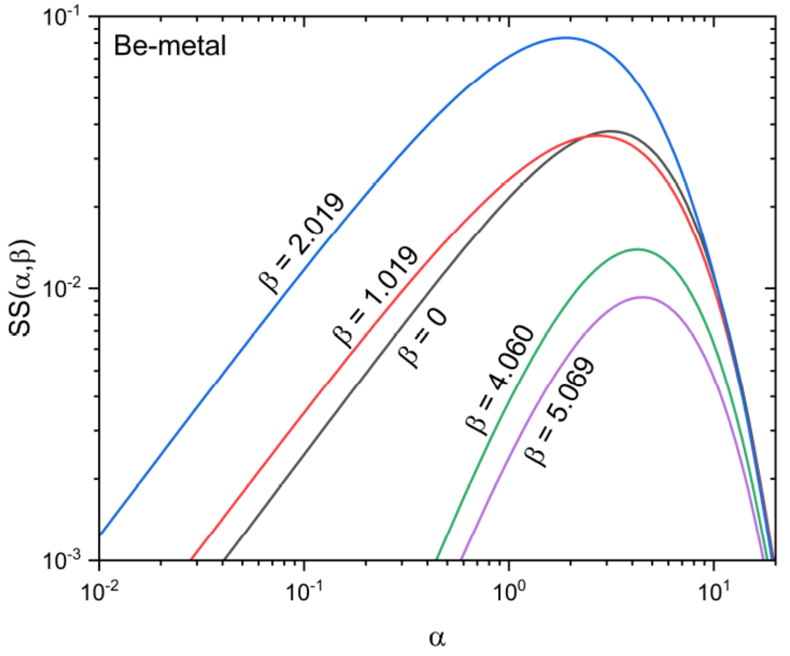
Advanced Moderators

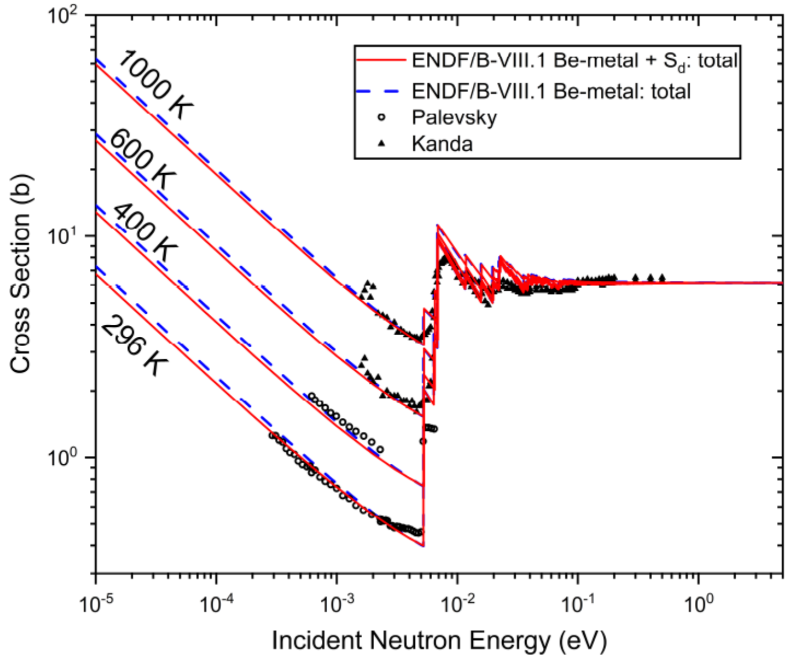
Material	Evaluator	Atomistic Method	New Physics	New Condition	Status
Be (metal)	NCSU	AILD	Sd, Exp. Lat. Param.		Reevaluation
BeO	NCSU	AILD	Exp. Lat. Param.		Reevaluation
ZrH_x, ZrH_2	NNL	AIMD/AILD	Mixed elastic, random alloy, Zr coherent elastic	Material phase dependent	New
YH_2	NNL	AILD	Mixed elastic, Exp. Lat. Param., Y coherent elastic		Reevaluation
ZrC	NNL	AILD	Mixed elastic, random alloy		New
Be_2C	NNL	AILD	Exp. Lat. Param.		New
^7LiH, ^7LiD	NNL	AILD	Mixed elastic, Exp. Lat. Param.		New
CaH_2	NCSU	AILD	2-Site H phonons, Exp. Lat. Param.		New

Be-metal

- Evaluations with *FLASSH* + AILD
  - 77, 100, 293.6, 296, 400, 500, 600, 700, 800, 1000 1200 K
- Reevaluation
  - MT2 changes due to use of exp lattice parameter
  - MT4 same model as ENDF/B-VIII.0
- New S_d evaluation
  - MT4 includes coherent inelastic
    - Same as ENDF/B-VIII.0 model otherwise

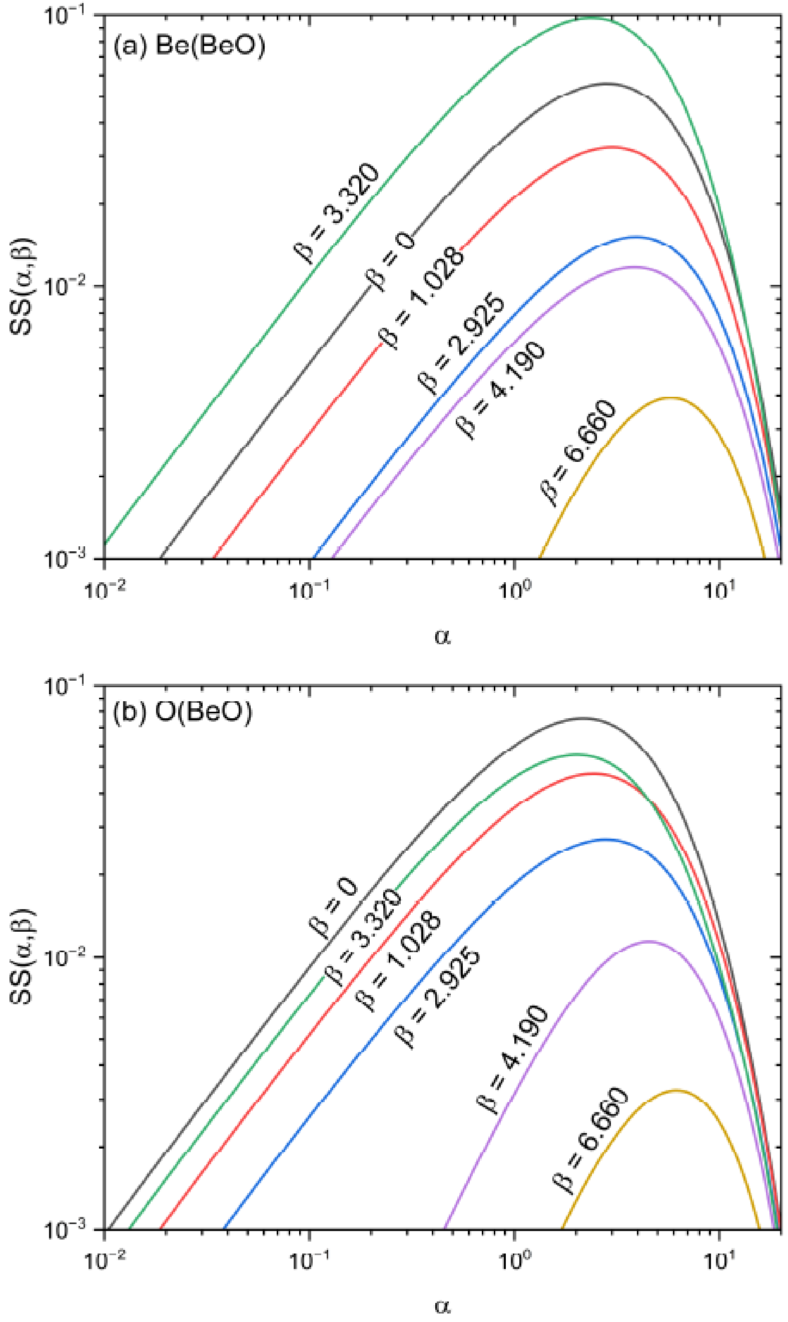


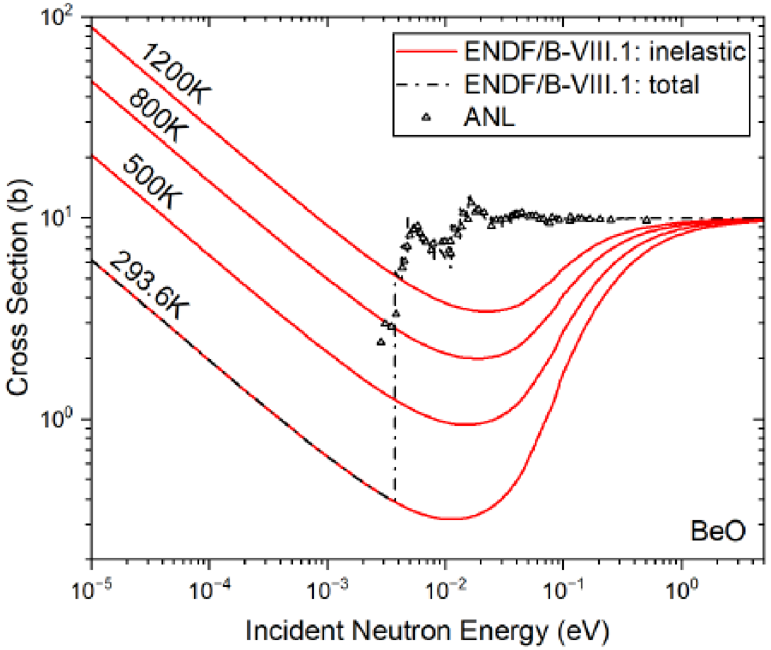




BeO

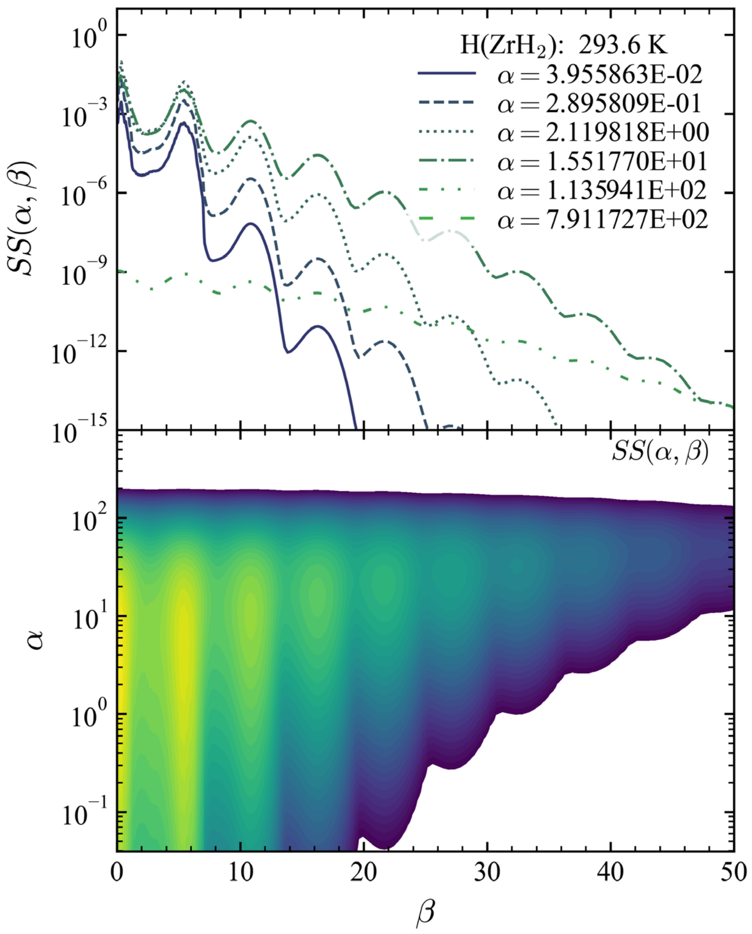
- Evaluations with *FLASSH* + AILD
  - 296, 400, 500, 600, 700, 800, 1000, 1200 K
- Reevaluation
  - Be(BeO) & O(BeO)
  - MT2 changes due to use of exp lattice parameter
  - MT4 same model as ENDF/B-VIII.0

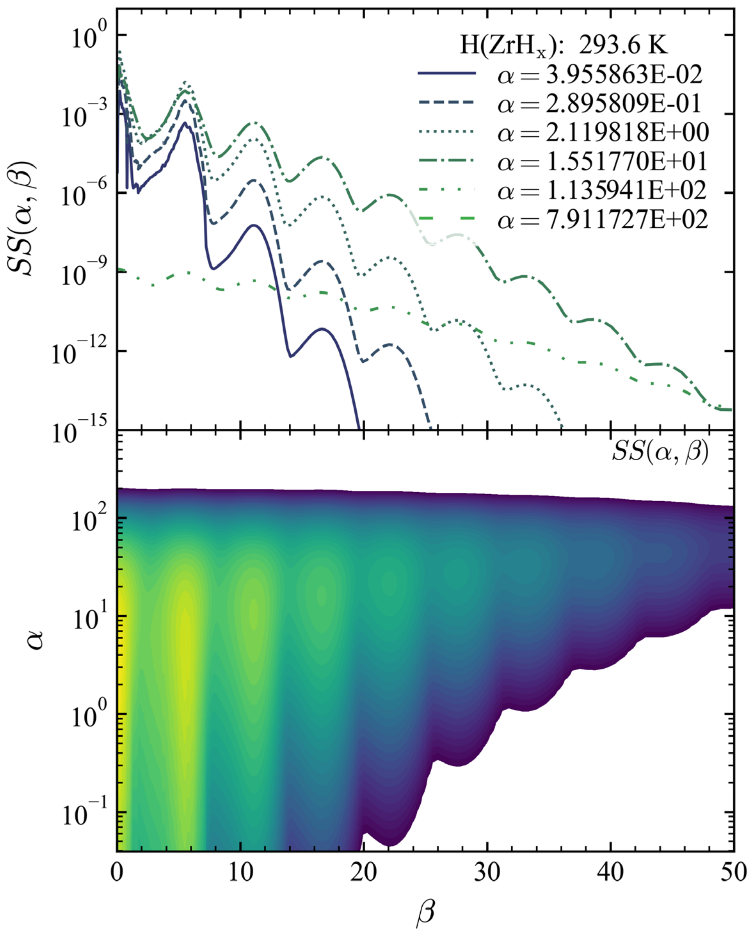




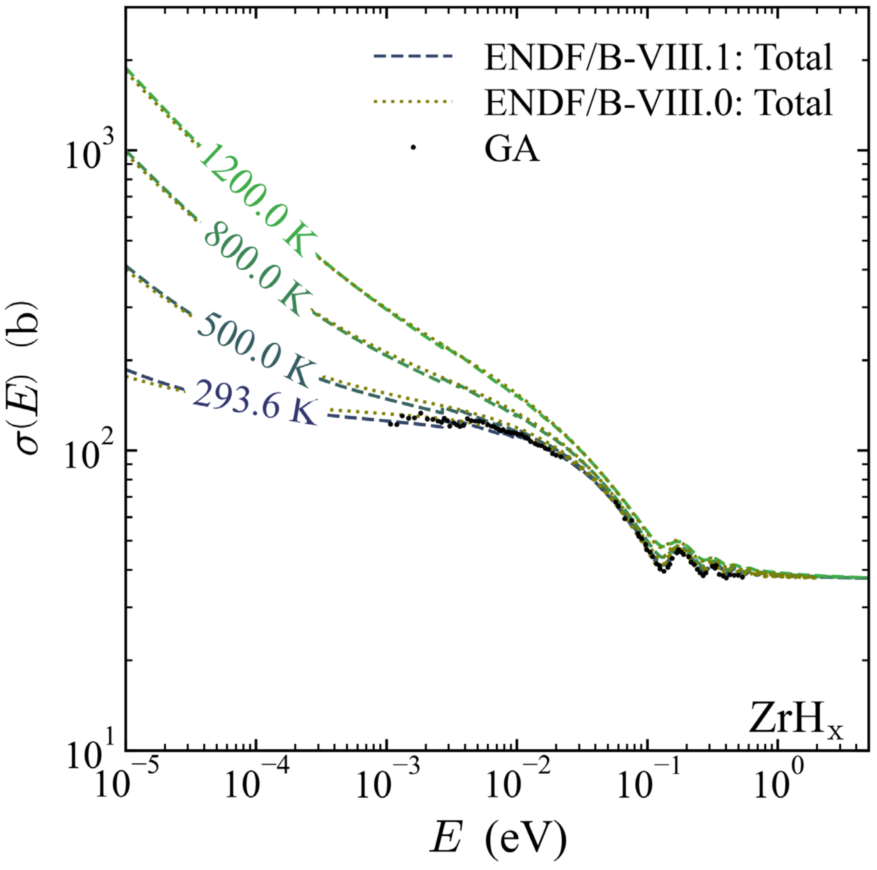
ZrH_x and ZrH_2

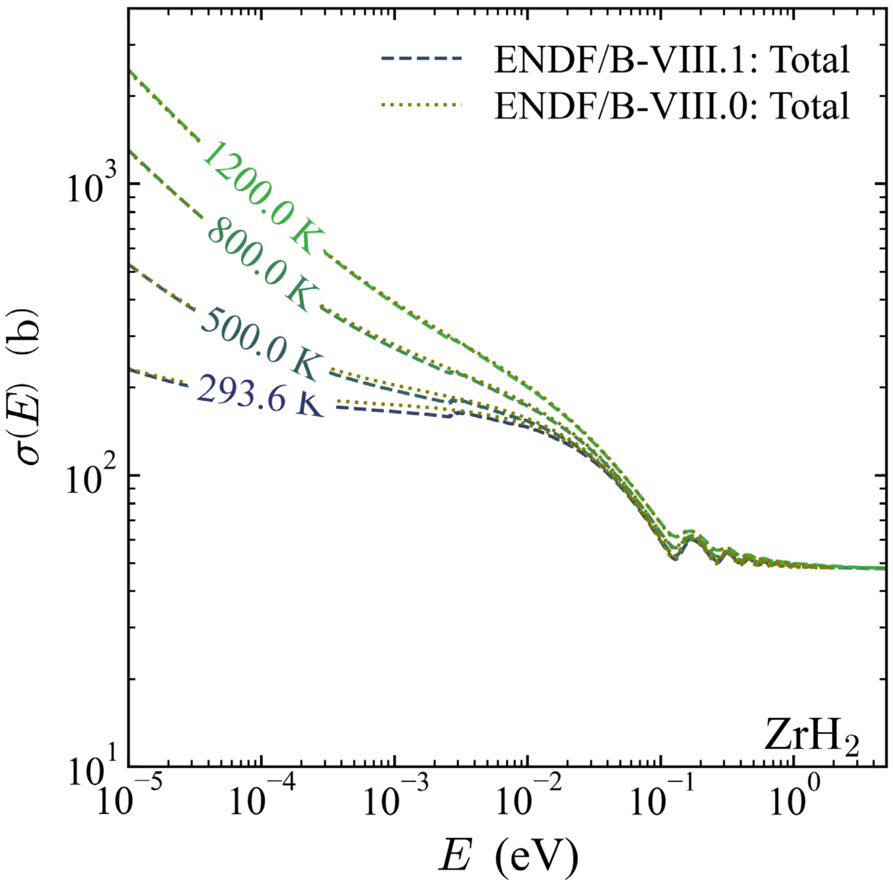
- Evaluations with *FLASSH* + AILD/AIMD
  - 77, 293.6, 400, 500, 600, 700, 800, 1000, 1200 K
- New evaluations
  - Alternative to ZrH with two phases of zirconium hydride treated separately
    - $H(ZrH_x)$ and $Zr(ZrH_x)$ for delta-phase
    - $H(ZrH_2)$ and $Zr(ZrH_2)$ for epsilon-phase)
  - Coherent elastic scattering added to MT2 $Zr(ZrH_x)$ and $Zr(ZrH_2)$
  - MT2 mixed elastic for Zr and incoherent elastic for H
  - MT4 AIMD for H; AILD for Zr





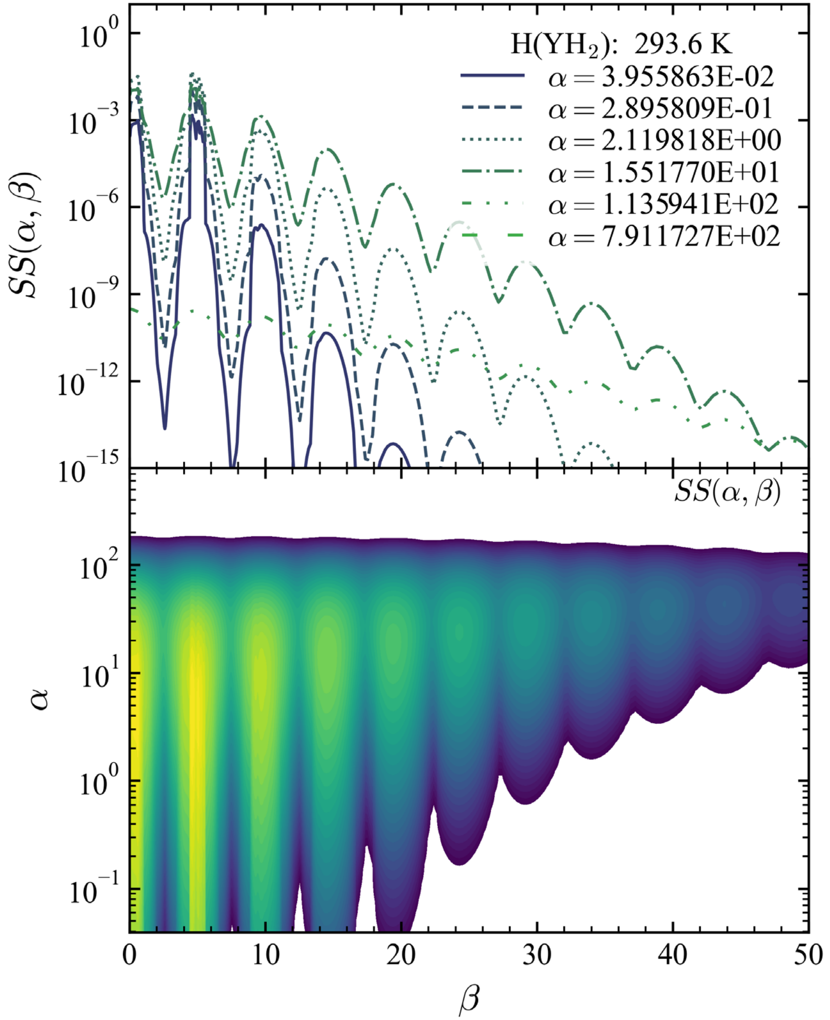
ZrH_x and ZrH_2 continued…

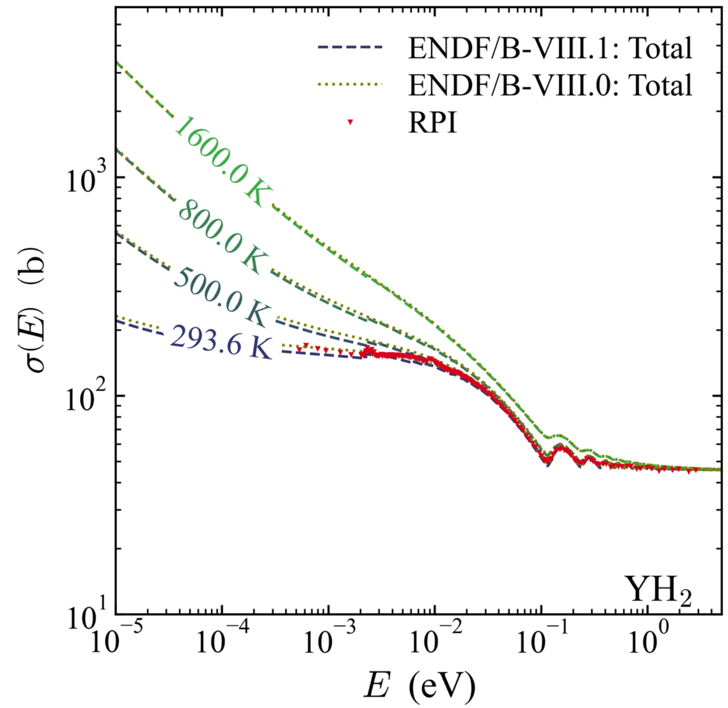




YH_2

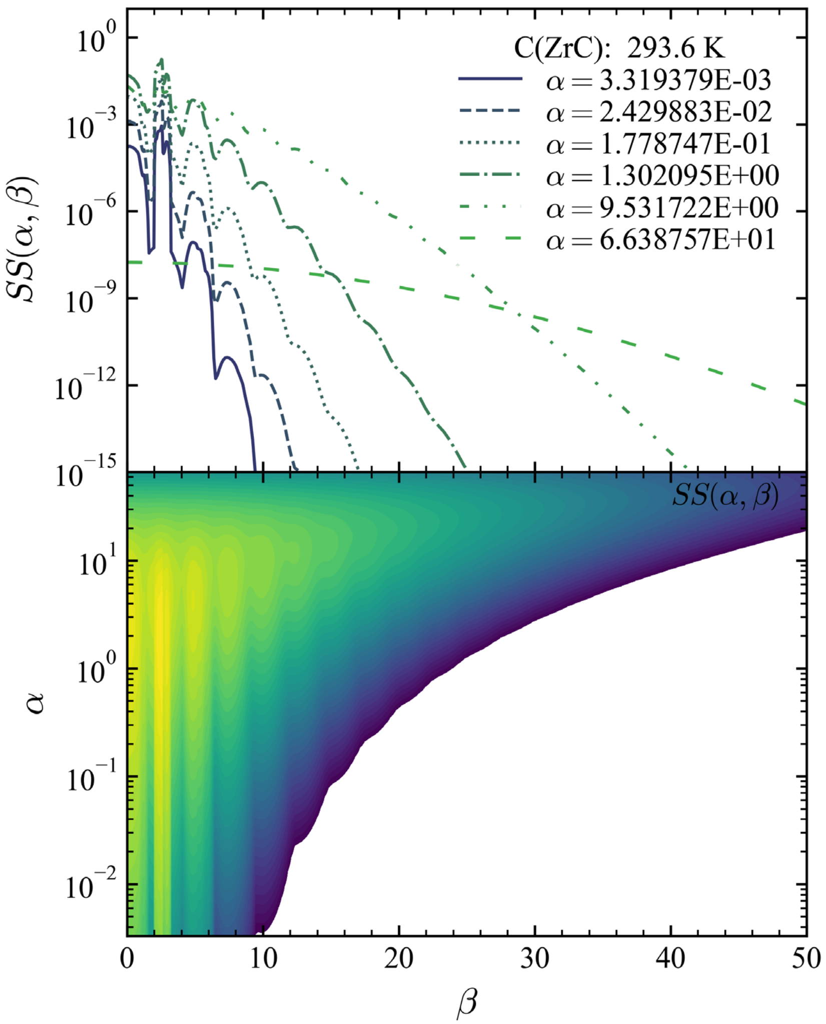
- Evaluations with *FLASSH* + AILD
  - 293.6, 400, 500, 600, 700, 800, 1200, 1400, 1600 K
- Reevaluation
  - MT2 added to $Y(YH_2)$
  - MT4 same model as ENDF/B-VIII.0 but new dense β to capture oscillations

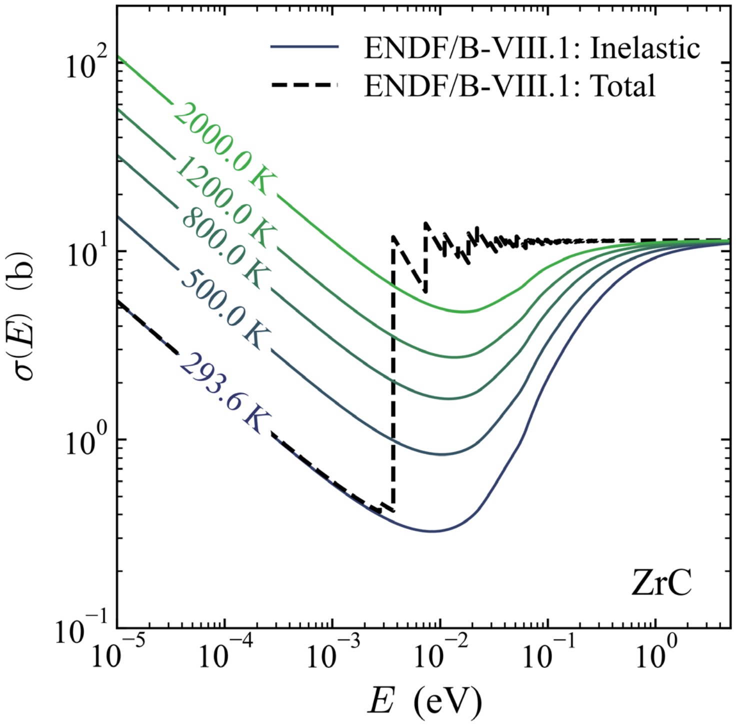




ZrC

- Evaluations with *FLASSH* + AILD
  - 77, 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1400, 1600, 1800, 2000 K
- New evaluation
  - C(ZrC) and Zr(ZrC)
  - Natural isotopic compositions
  - MT2 mixed elastic
    - Random alloy theory in coherent elastic for isotopic composition
  - MT4 of C(ZrC) exhibits oscillations typical of metal-hydrides



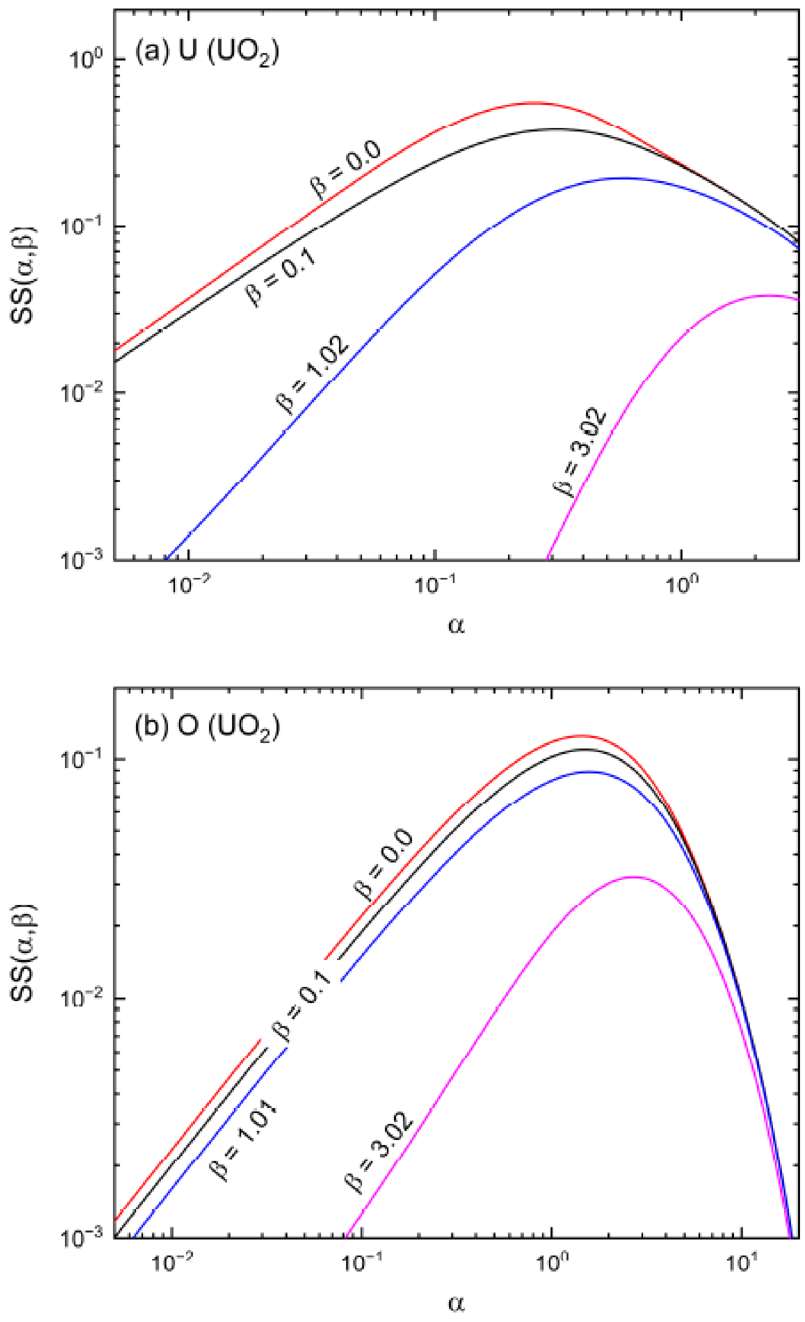


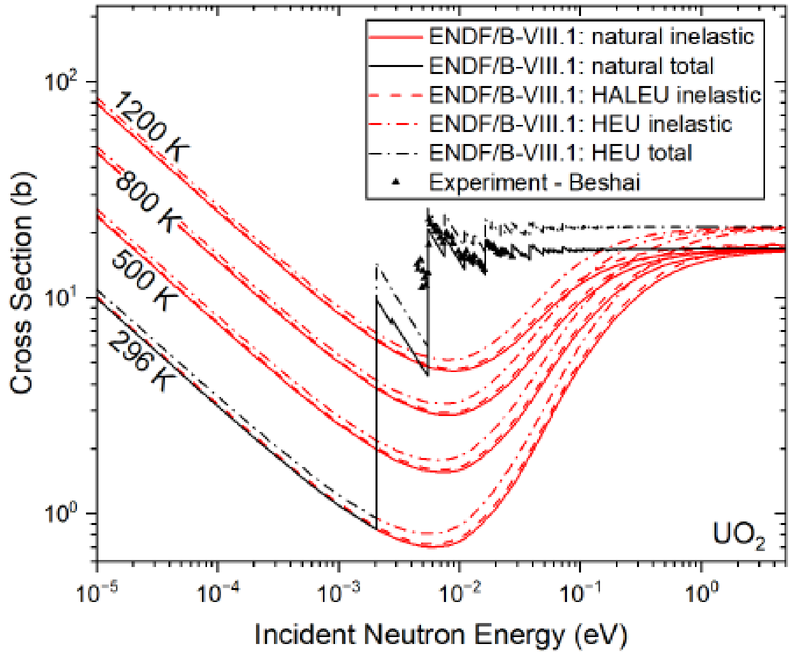
Fuel Compounds

Material	Evaluator	Atomistic Method	New Physics	New Condition	Status
UO_2	NCSU	AILD	Exp. Lat. Param.	^{235}U enrichment	Reevaluation
UN	NCSU	AILD	Exp. Lat. Param.	^{235}U enrichment	Reevaluation
UC	NCSU	AILD	Exp. Lat. Param	^{235}U enrichment	New
U (metal)	NCSU	MD-LD	Exp. Lat. Param	^{235}U enrichment	New

UO_2

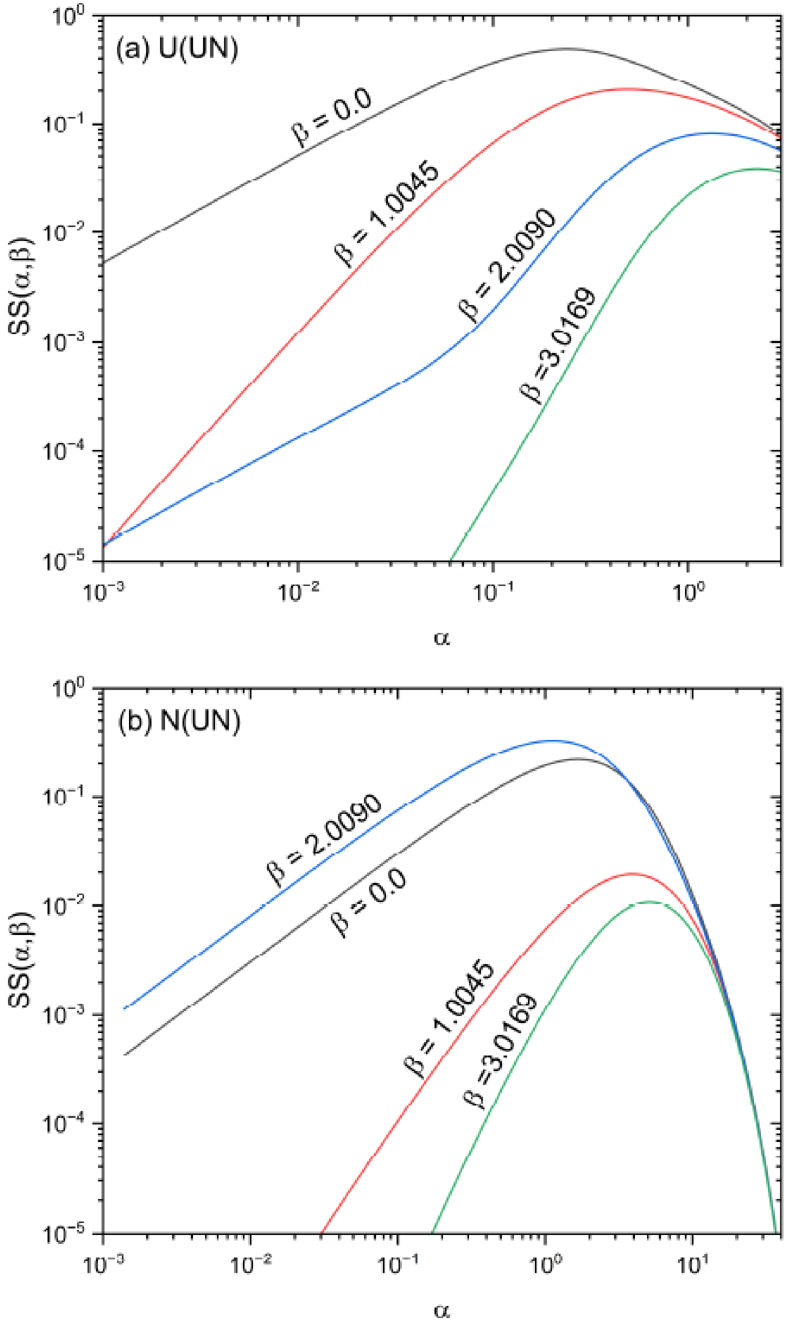
- Evaluations with *FLASSH* + AILD
  - 296, 400, 500, 600, 700, 800, 1000, 1200 K
- Reevaluation
  - $O(UO_2)$ and $U(UO_2)$
  - Same material model as ENDF/B-VIII.0
  - MT2 uses exp lattice parameter
  - Enrichments: natural, 5%, 10%, 19.75%, 93%, 100%

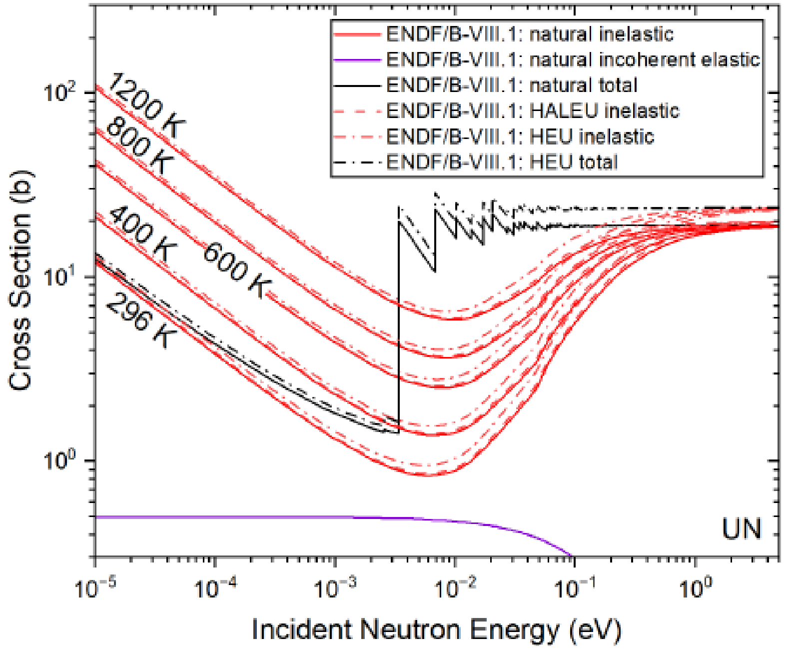




UN

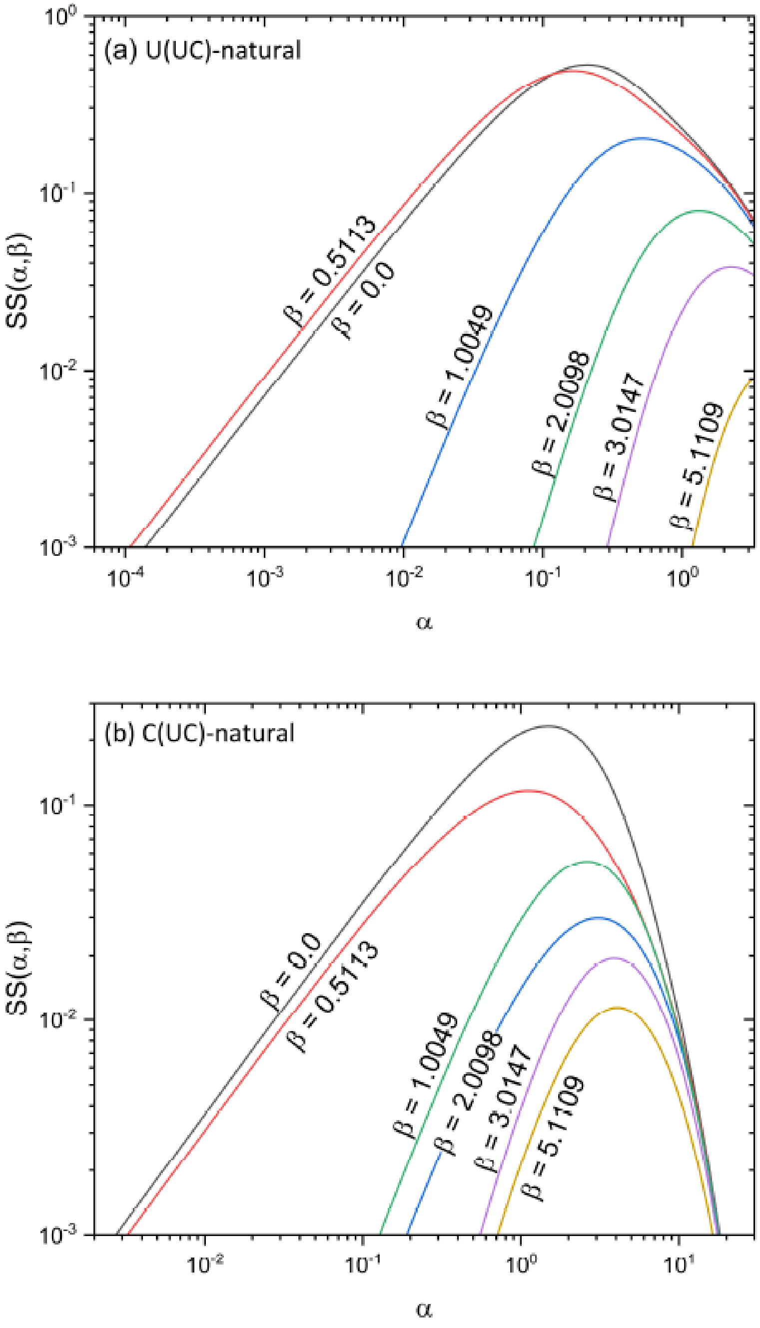
- Evaluations with *FLASSH* + AILD
  - 296, 400, 500, 600, 700, 800, 1000, 1200 K
- Reevaluation
  - N(UN) and U(UN)
  - Same material model as ENDF/B-VIII.0
  - Enrichments: natural, 5%, 10%, 19.75%, 93%, 100%

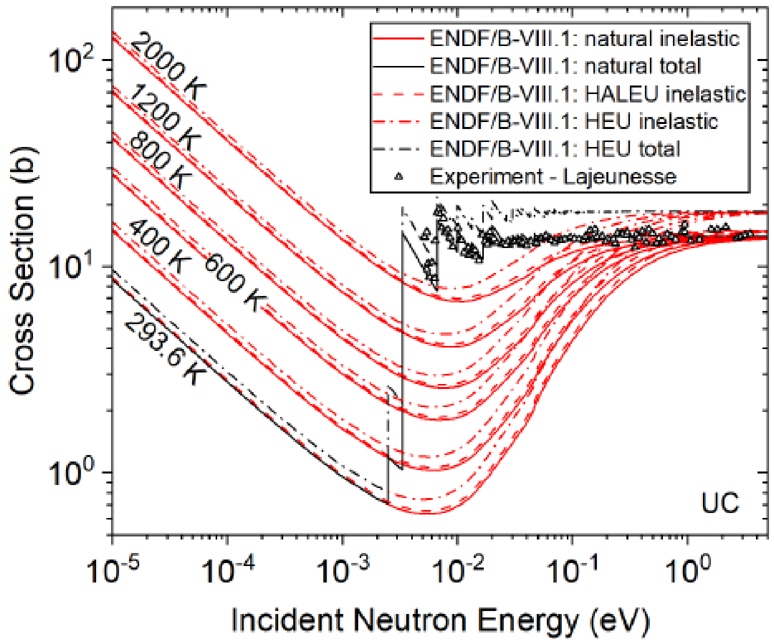




UC

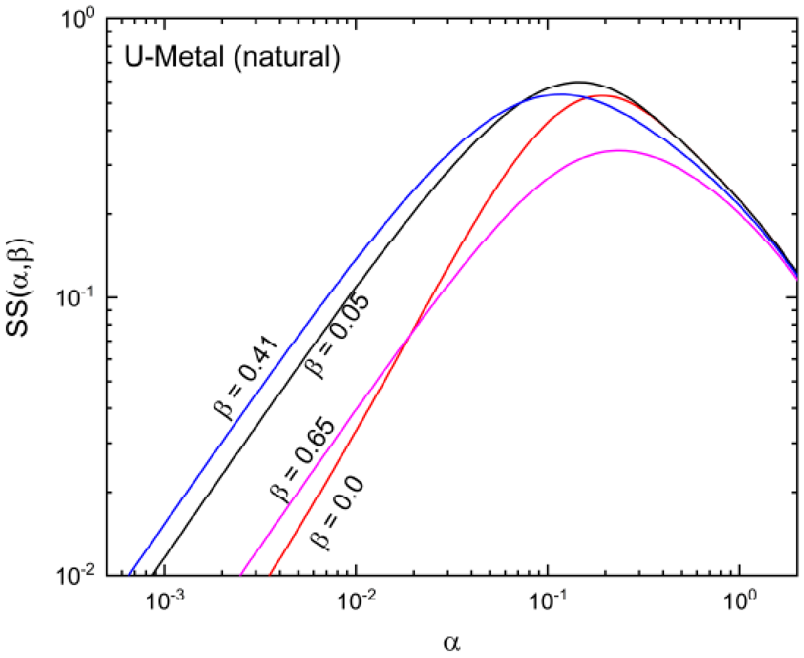
- Evaluations with *FLASSH* + AILD
  - 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000 K
- New Evaluation
  - C(UC) and U(UC)
  - Enrichments: natural, 5%, 10%, 19.75%, 93%, 100%

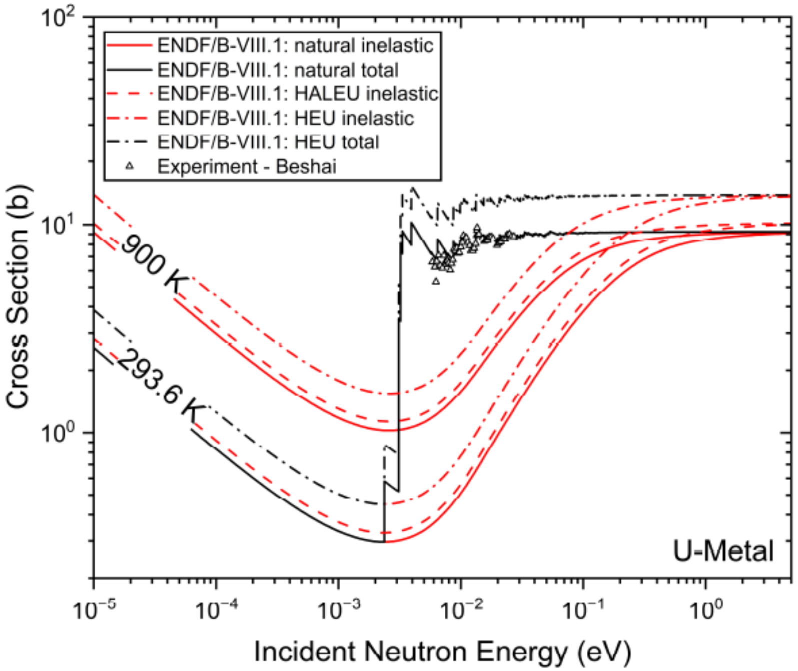




U-metal

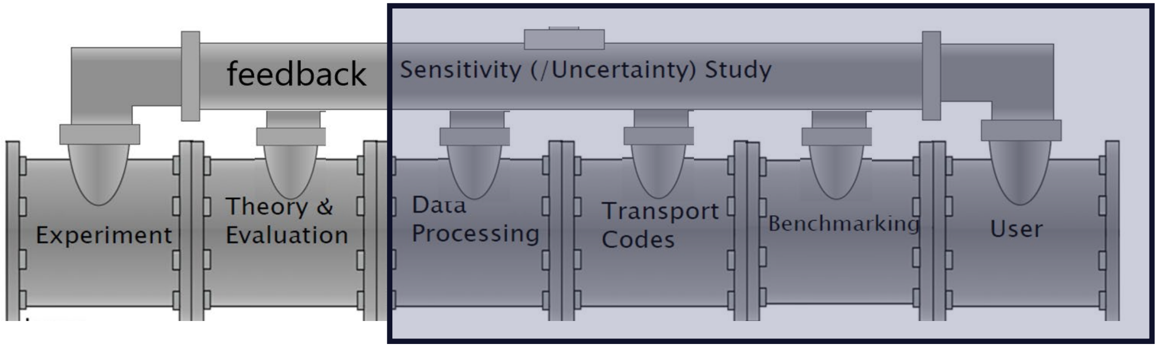
- Evaluations with *FLASSH* + MD-LD
  - 296, 400, 500, 600, 700, 800, 900 K
- New Evaluation
  - Enrichments: natural, 5%, 10%, 19.75%, 93%, 100%





Nuclear Data Pipeline – Where We Are & Call for Action

Where We Are



- Theory & TSL Evaluation tools in place to drive continued innovation
- Additional improvements planned by CSEWG TSL evaluators

What's needed now?

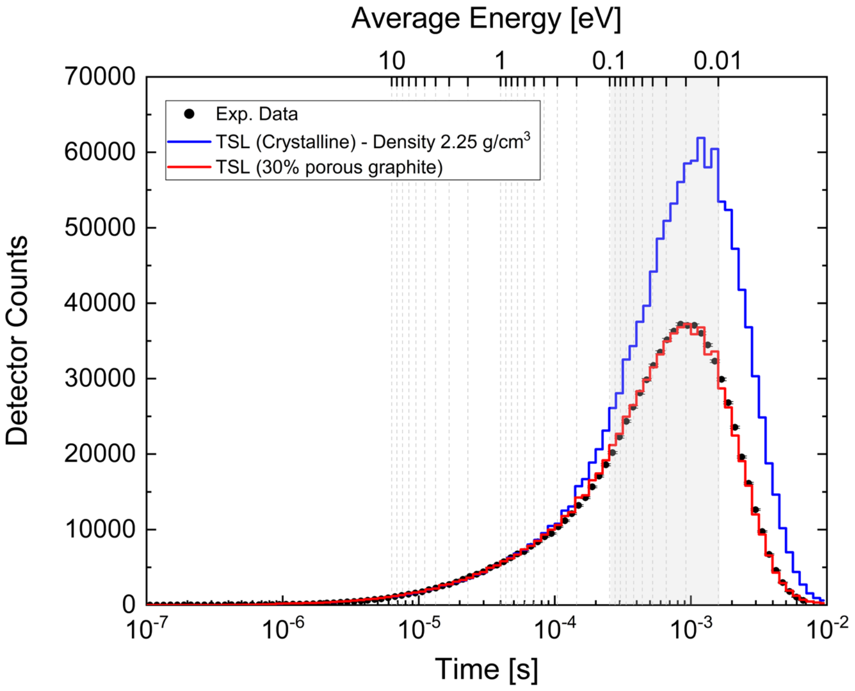
- Industry & national lab user feedback on TSLs
- **Validation benchmarks**
  - Critical Experiments
  - Reactor startup data
  - Diffusion (PNDA) experiments
  - **TRISO benchmarks**
    - **Proper attention to TRISO self-shielding effects in prototypical fuel element configurations essential**

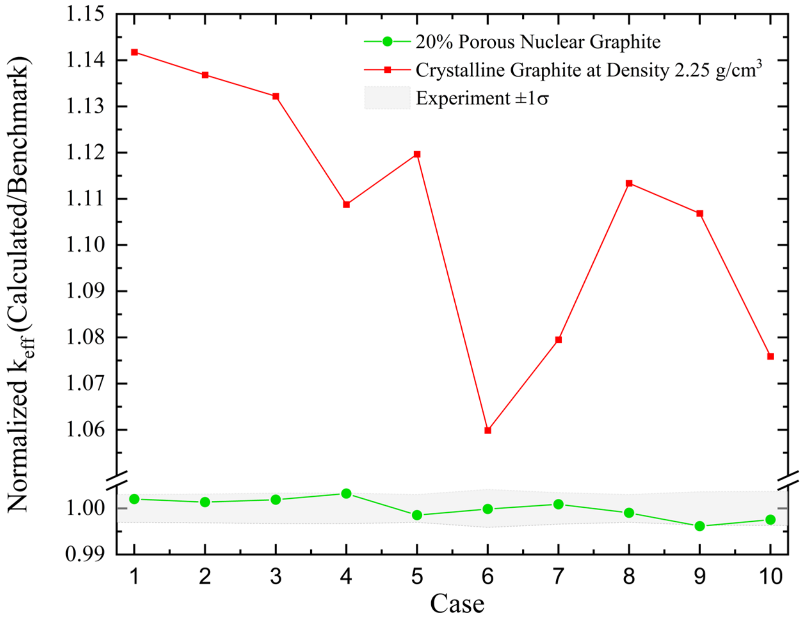
Backup

Modeling with Consistent Graphite Density

- ORELA and PROTEUS without historical density approximation (2.25 g/cm^3)

Self-consistent phonon DOS and density





From Ayman Hawari's Graphite History Presentation at 2024 NCSP TRP