Technical Program Review
Nuclear Criticality Safety Program
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Progress of Thermal Scattering Law Development and Evaluations at North Carolina State University

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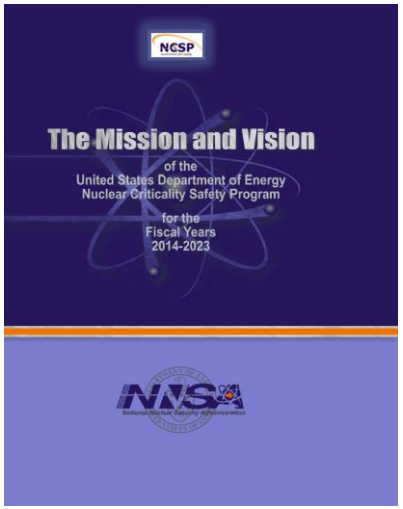
Acknowledgement

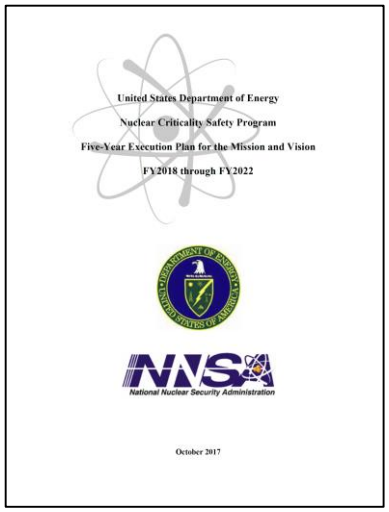
- The many graduate students, postdocs, and research staff at North Carolina State University
- Collaboration with LLNL and Bettis labs
  - David Heinrichs, Michael Zerkle, Jesse Holmes
- Funding
  - US NNSA Nuclear Criticality Safety program
  - US Naval Nuclear Propulsion Program

FY 2018/2019

- 4 new TSL evaluations
  - 3 first-of-a-kind evaluations
- Modern predictive methods for thermal neutron cross section calculations based on the use of atomistic simulations
  - Ab initio lattice dynamics
  - Molecular dynamics (ab initio and classical)
    - New materials
    - All states of matter (solid, liquid, gas)
    - Imperfect structure
- Expanding the *FLASSH* thermal scattering analysis platform
  - Removed approximations such as incoherent approximation, cubic approximation, atom site approximation and SCT approximation
- Initiated the integration of the Generalized Nuclear Data Structure (GNDS) format into *FLASSH*

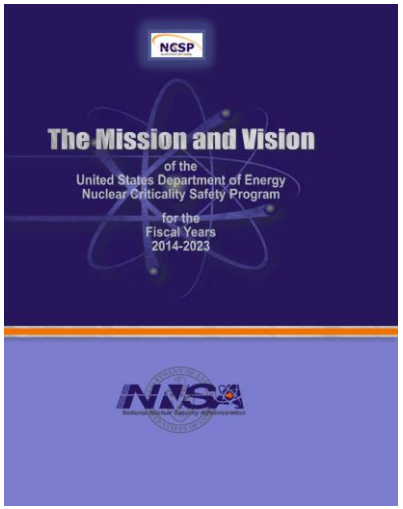
Objectives

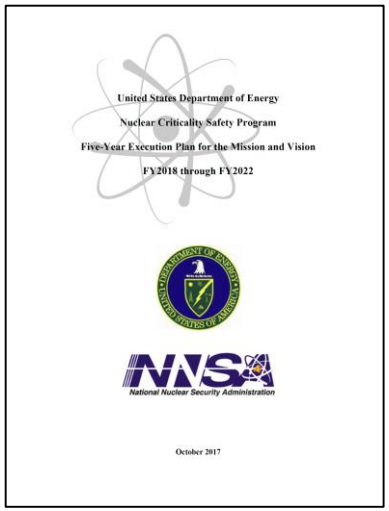




Priority Needs */ **Additional Needs**	Thermal scattering (Paraffinic Oil, HF, Silicone Oil, UO_2F_2, PuH_2, UH_3, Paraffin, U_3O_8, U_3Si_2, UC, PuO_2, etc.), ^{239}Pu, Fe, Cr, ^{237}Np, Pb, ^{55}Mn, Ti, ^{240}Pu/ ^{233}U, Th, Be, ^{51}V, Zr, F, K, Ca, Mo, Na, La
Completed Evaluations (FY)	Minor Actinides (13), SiC(17), SiO_2 (17), $C_5O_2H_8$ (16), CH_2 (17), Be (17), BeO (17), Graphite (17), UO_2 (17), UN (17), ^{55}Mn (12), ^{58,60}Ni (14), ^{180,128,183,184,186}W (14), Ca (16), ^{59}Co (17), ^{63,65}Cu(17)

Objectives





Priority Needs */ Additional Needs	Thermal scattering (Paraffin, Oil, HF, Silicone Oil, UO_2F_2, PuH_2, UH_3, Paraffin, U_3O_8, U_3Si_2, UC, PuO_2, etc.), ^{239}Pu, Fe, Cr, ^{237}Np, Pb, ^{55}Mn, Ti, ^{240}Pu/^{233}U, Th, ^{51}V, Zr, F, K, Ca, Mo, Na, La
Completed Evaluations (FY)	Minor Actinides (13), Si (17), Si (17), $C_5O_2H_8$ (16), C (17), Be (17), B (17), Graphite (17), U (17), B (17), ^{55}Mn (12), ^{58,60}Ni (14), ^{180,128,183,184,186}W (14), Ca (16), ^{59}Co (17), ^{63,65}Cu(17)

Completed light water (H_2O)

Finalizing molten salt FLiBe

Neutron Thermalization

Using first Born approximation combined with Fermi pseudopotential, it can be shown that the double differential scattering cross section has the form

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi}\sqrt{\frac{E'}{E}}\left\{\sigma_{coh}S(\vec{\kappa},\omega) + \sigma_{incoh}S_s(\vec{\kappa},\omega)\right\}$$

The scattering law $S(\vec{\kappa},\omega)$ is composed of two parts

$$S(\vec{\kappa},\omega) = S_s(\vec{\kappa},\omega) + S_d(\vec{\kappa},\omega)$$

Van Hove's space-time formulation

$$I(\vec{\kappa},t) = \int G(\vec{r},t)\exp(i\vec{\kappa}\cdot\vec{r})d\vec{r}$$

$$S(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(\vec{r},t)e^{i(\vec{\kappa}\cdot\vec{r}-\omega t)}d\vec{r}dt$$

where $G(\vec{r},t)$ is the *dynamic pair correlation function* and can be expressed in terms of time dependent atomic positions.

Since 1960s
GASKET
NJOY/LEAPR
INCOHERENT
APPROXIMATION

$$S_s(\alpha,\beta) = k_B T \cdot S_s(\vec{\kappa},\omega)$$

$$\left.\frac{d^2\sigma}{d\Omega dE'}\right|_{inelastic} = \frac{\sigma}{2k_B T}\sqrt{\frac{E'}{E}}S_s(\alpha,\beta)$$

$\beta = \frac{E - E'}{k_B T}$ Energy transfer

$\alpha = \frac{(E + E' - 2\sqrt{EE'}\cos\theta)}{k_B T}$ Momentum transfer

The scattering law (TSL) is the Fourier transform of a Gaussian correlation function

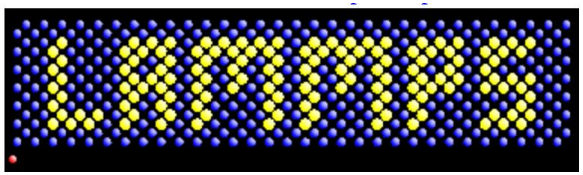
$$S_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\beta t} e^{-\gamma(t)} dt$$

$$\gamma(t) = \frac{\alpha}{2}\int_{-\infty}^{\infty} \frac{\rho(\beta)}{\beta \sinh(\beta/2)}\left[1 - e^{-i\beta t}\right] e^{\beta/2} d\beta$$

$\rho(\beta)$ – density of states (e.g., phonon frequency distribution)

Thermal Scattering Law Analysis

- Key development in the last 20 years is the use of atomistic simulations methods to support the evaluation process
  - Produce data necessary to calculate the TSL including
    - DOS for evaluation of TSL
    - Direct access to TSL using correlation analysis



ENDF/B-VIII TSL Evaluations

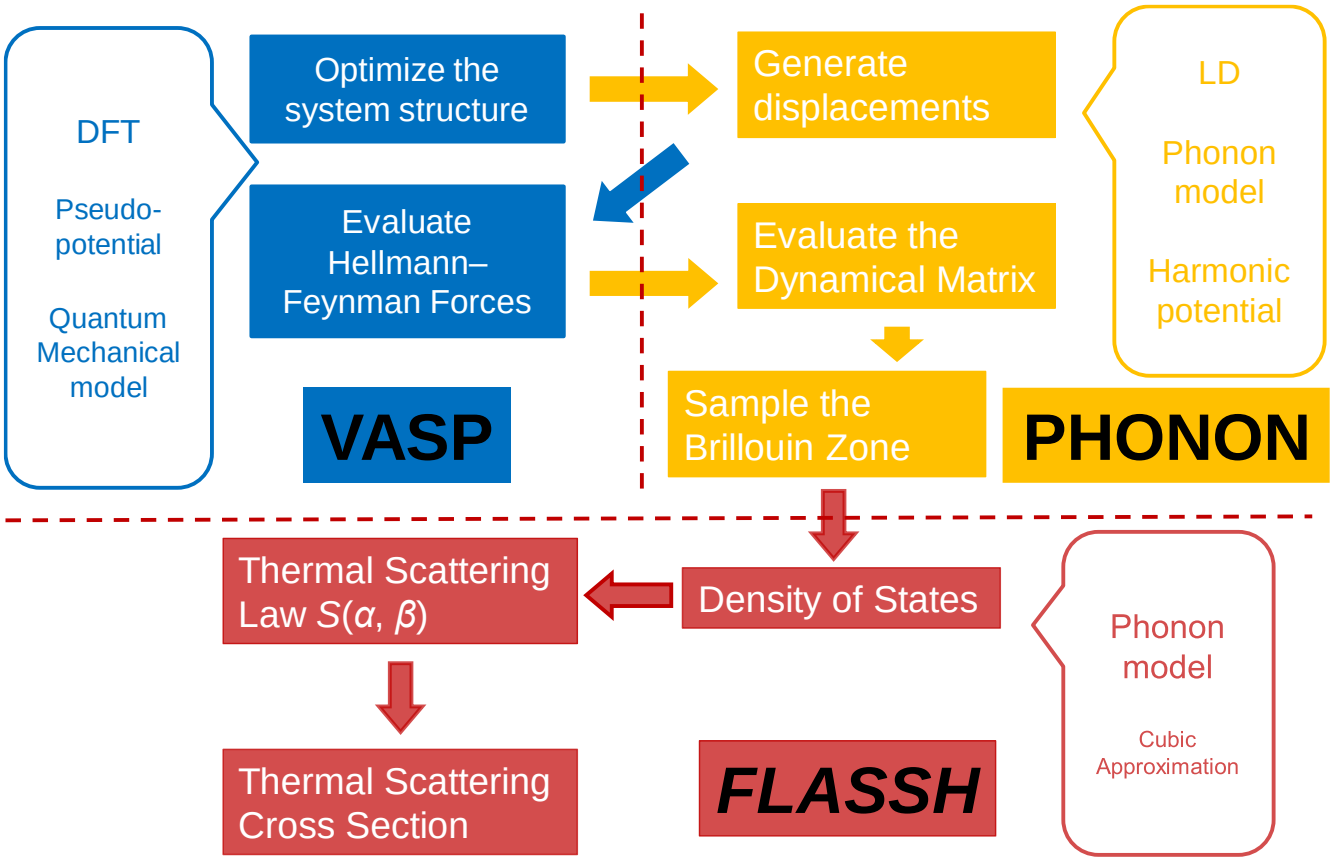
Material	ENDF Library Name	Evaluation Basis	Institution
Beryllium metal	tsl-Be-metal.endf	DFT/LD	NCSU
Beryllium oxide (beryllium)	tsl-BeinBeO.endf	DFT/LD	NCSU
Beryllium oxide (oxygen)	tsl-OinBeO.endf	DFT/LD	NCSU
Light water (hydrogen)	tsl-HinH2O.endf	MD	CAB
Light water ice (hydrogen)	tsl-HinIceIh.endf	DFT/LD	BAPL
Light water ice (oxygen)	tsl-OinIceIh.endf	DFT/LD	BAPL
Heavy water (deuterium)	tsl-DinD2O.endf	MD	CAB
Heavy water (oxygen)	tsl-OinD2O.endf	MD	CAB
Polymethyl Methacrylate (Lucite)	tsl-HinC5O2H8.endf	MD	NCSU
Polyethylene	tsl-HinCH2.endf	MD	NCSU
Crystalline graphite	tsl-graphite.endf	MD	NCSU
Reactor graphite (10% porosity)	tsl-reactor-graphite-10P.endf	MD	NCSU
Reactor graphite (30% porosity)	tsl-reactor-graphite-30P.endf	MD	NCSU
Silicon carbide (silicon)	tsl-CinSiC.endf	DFT/LD	NCSU
Silicon carbide (carbon)	tsl-SiinSiC.endf	DFT/LD	NCSU
Silicon dioxide (alpha phase)	tsl-SiO2-alpha.endf	DFT/LD	NCSU
Silicon dioxide (beta phase)	tsl-SiO2-beta.endf	DFT/LD	NCSU
Yttrium hydride (hydrogen)	tsl-HinYH2.endf	DFT/LD	BAPL
Yttrium hydride (yttrium)	tsl-YinYH2.endf	DFT/LD	BAPL
Uranium dioxide (oxygen)	tsl-OinUO2.endf	DFT/LD	NCSU
Uranium dioxide (uranium)	tsl-UinUO2.endf	DFT/LD	NCSU
Uranium nitride (nitrogen)	tsl-NinUN.endf	DFT/LD	NCSU
Uranium nitride (uranium)	tsl-UinUN.endf	DFT/LD	NCSU

ENDF/B-VIII TSL Evaluations

Material	ENDF Library Name	Evaluation Basis	Institution
Beryllium metal	tsl-Be-metal.endf	DFT/LD	NCSU
Beryllium oxide (beryllium)	tsl-BeinBeO.endf	DFT/LD	NCSU
Beryllium oxide (oxygen)	tsl-OinBeO.endf	DFT/LD	NCSU
Light water (hydrogen)	tsl-HinH2O.endf	MD	CAB
Light water ice (hydrogen)	tsl-HinIceIh.endf	DFT/LD	BAPL
Light water ice (oxygen)	tsl-OinIceIh.endf	DFT/LD	BAPL
Heavy water (deuterium)	tsl-DinD2O.endf	MD	CAB
Heavy water (oxygen)	tsl-OinD2O.endf	MD	CAB
Polymethyl Methacrylate (Lucite)	tsl-HinC5O2H8.endf	MD	NCSU
Polyethylene	tsl-HinCH2.endf	MD	NCSU
Crystalline graphite	tsl-graphite.endf	MD	NCSU
Reactor graphite (10% porosity)	tsl-reactor-graphite-10P.endf	MD	NCSU
Reactor graphite (30% porosity)	tsl-reactor-graphite-30P.endf	MD	NCSU
Silicon carbide (silicon)	tsl-CinSiC.endf	DFT/LD	NCSU
Silicon carbide (carbon)	tsl-SiinSiC.endf	DFT/LD	NCSU
Silicon dioxide (alpha phase)	tsl-SiO2-alpha.endf	DFT/LD	NCSU
Silicon dioxide (beta phase)	tsl-SiO2-beta.endf	DFT/LD	NCSU
Yttrium hydride (hydrogen)	tsl-HinYH2.endf	DFT/LD	BAPL
Yttrium hydride (yttrium)	tsl-YinYH2.endf	DFT/LD	BAPL
Uranium dioxide (oxygen)	tsl-OinUO2.endf	DFT/LD	NCSU
Uranium dioxide (uranium)	tsl-UinUO2.endf	DFT/LD	NCSU
Uranium nitride (nitrogen)	tsl-NinUN.endf	DFT/LD	NCSU
Uranium nitride (uranium)	tsl-UinUN.endf	DFT/LD	NCSU

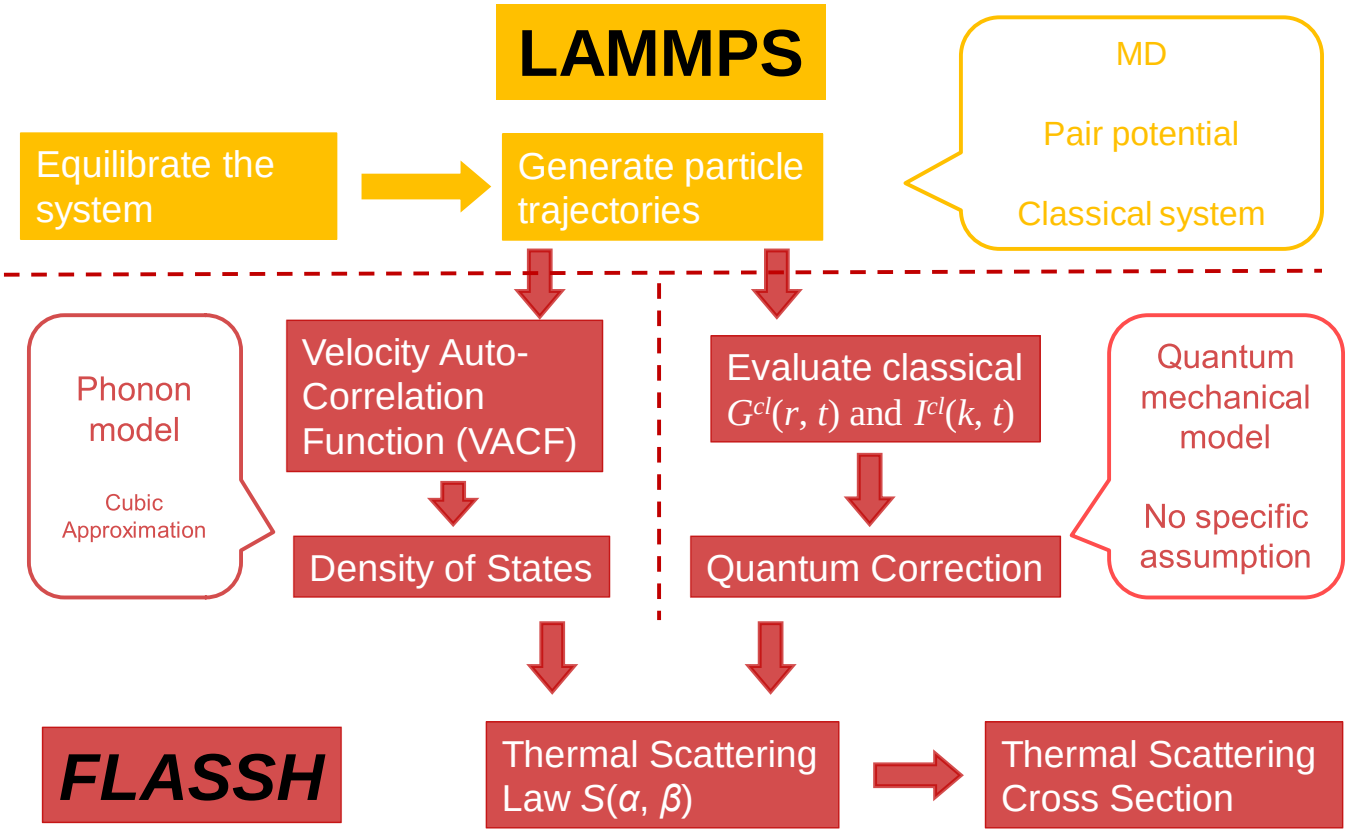
Thermal Scattering Cross-Sections

Evaluation DFT/LD



Thermal Scattering Cross-Sections

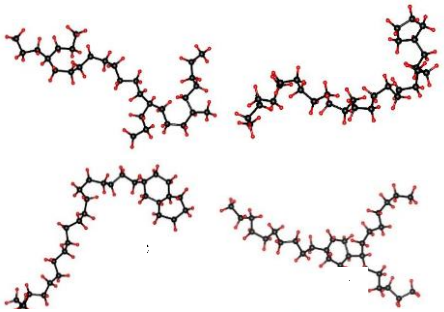
Evaluation MD/QM

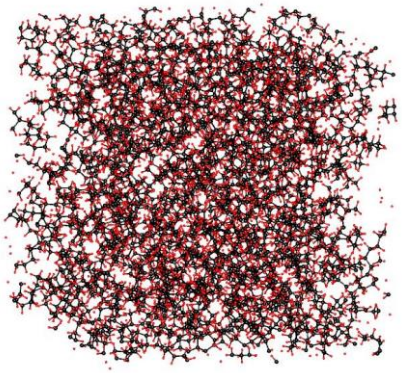


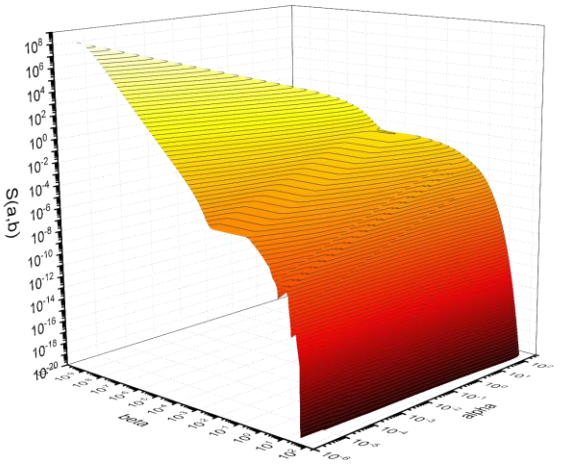
Computational Capabilities

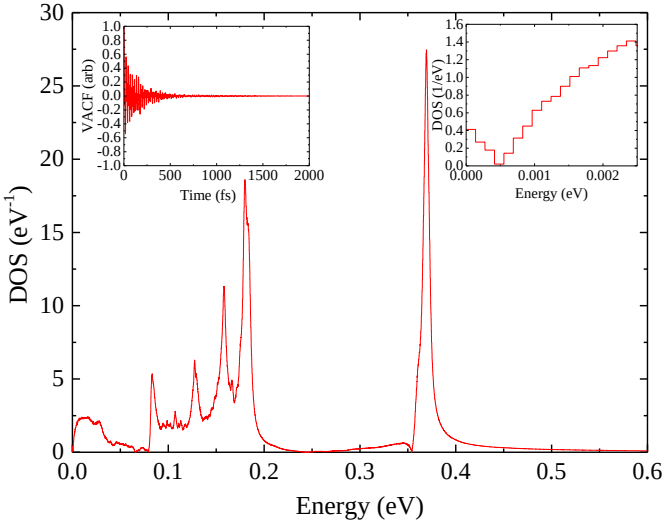
- Hybrid mini cluster - 17 nodes
  - 324 CPU cores
  - 22 Nvidia GPUs
  - Expanding…..
- Parallel computations
  - Atomistic simulations
  - TSL analysis
  - Neutronic simulations
  - System design
- VASP, PHONON, LAMMPS PREPRO, NJOY, FUDGE, SAMMY, MCNP, Serpent, GEANT4, McStas, PARET, RELAP, COMSOL

Heavy Paraffinic Oil







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0.000000+0 0.000000+0           0           0           0           6  38 1451    2
1.000000+0 5.000000+0           0           0          12           8  38 1451    3
0.000000+0 0.000000+0           0           0          34           2  38 1451    4
H(Paraffinic Oil) LEIP LAB  EVAL-SEP17 C.A. Manring, A.I. Hawari      38 1451    5
                                  DIST-                                38 1451    6
---ENDF/B-VIII.1      MATERIAL   38                                     38 1451    7
----THERMAL NEUTRON SCATTERING DATA                                     38 1451    8
-----ENDF-6 FORMAT                                                      38 1451    9
                                                                        38 1451   10
Temperatures = 300 K                                                    38 1451   11
                                                                        38 1451   12
Background                                                              38 1451   13
----------                                                              38 1451   14
                                                                        38 1451   15
This library was produced by the Low Energy Interactions Physics        38 1451   16
(LEIP) group at North Carolina State University.  A single              38 1451   17
temperature is available in this library.  The inelastic                38 1451   18
scattering cross section libraries for H in Paraffinic oil              38 1451   19
were developed using molecular dynamics methods [1]. This               38 1451   20
material is a viscous liquid polymer, such that the diffusion           38 1451   21
contribution to the TSL is not expected to be large. The                38 1451   22
diffusive behavior of the TSL for the current evaluation was            38 1451   23
approximated as a Langevin fluid of oil molecules with an average       38 1451   24
molecular mass of 421 amu.  Due to the fact that the quasi-             38 1451   25
elastic scattering peak is included in the TSL, only MT = 4 is          38 1451   26
tabulated in File 7.  The LEAPR module of the NJOY2016 code             38 1451   27
system was used to produce the MT = 4 data.  To avoid confusion         38 1451   28
with other materials, MAT 38 and ZA 138 were used for                   38 1451   29
H(Paraffinic Oil).                                                      38 1451   30
                                                                        38 1451   31
References                                                              38 1451   32
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                                                                        38 1451   34
1. A.I. Hawari, "Modern Techniques in Inelastic Thermal Neutron         38 1451   35
   Scattering Analysis," Nuclear Data Sheets 118 (2014) 172.            38 1451   36
                                                                        38 1451   37
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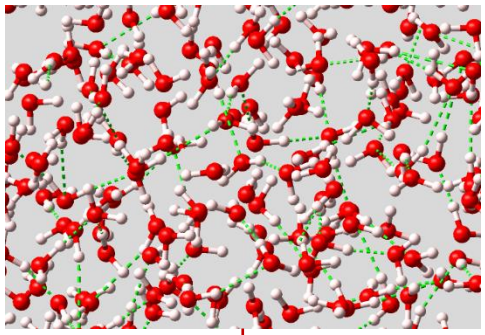
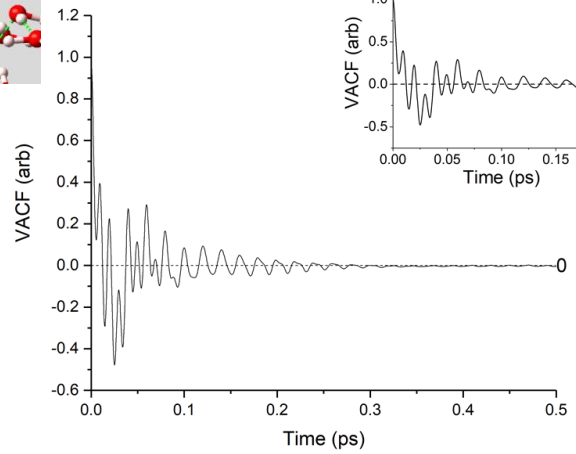
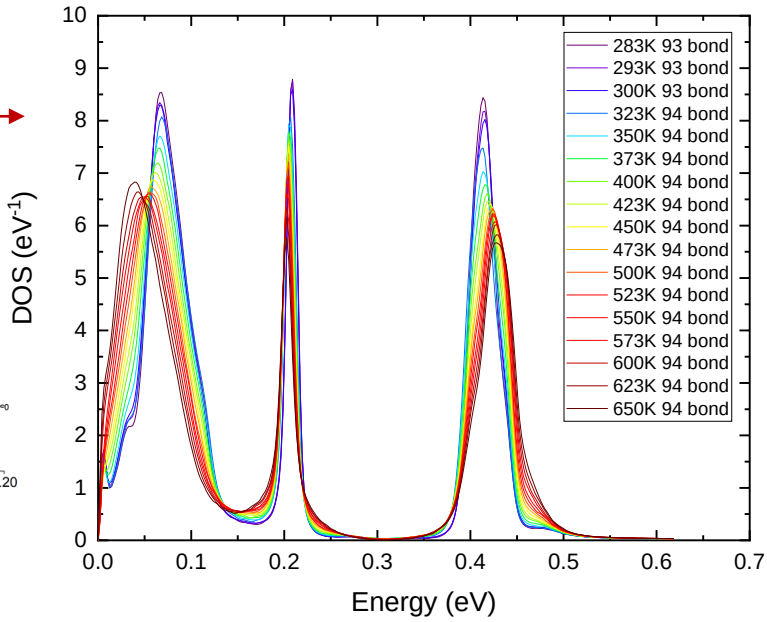
Light Water

Flexible TIP4P/2005 potential

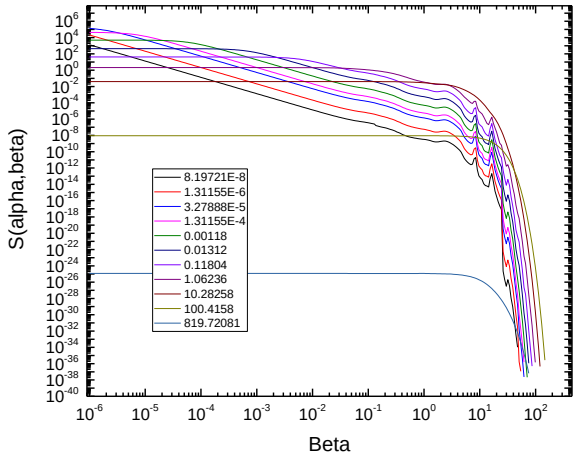
$$U^{tot} = U^{inter} + U^{intra} = \sum_{i \neq j} 4\varepsilon \left[\left(\frac{\sigma}{r_{O_i O_j}} \right)^{12} - \left(\frac{\sigma}{r_{O_i O_j}} \right)^{6} \right] + \sum_{i \neq j} \frac{q_i q_j}{r_{ij}} + D_r \left\{ 1 - \exp\left[-\beta (r_{OH} - r_{eq}) \right] \right\}^2 + \frac{1}{2} K_\theta (\theta - \theta_{eq})^2$$

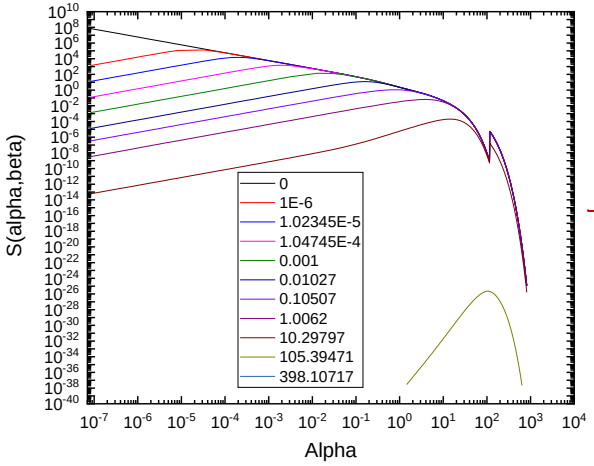


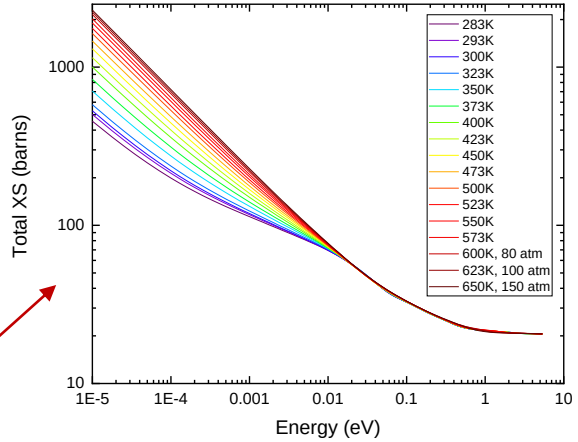


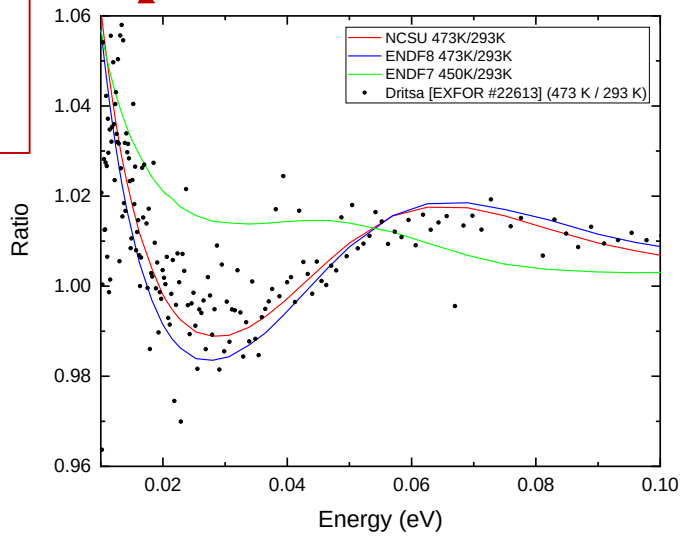


Light Water









File 7

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1.001000+3 9.991673-1          -1          0          0          0  1 1451    1
0.000000+0 0.000000+0           0          0          0          6  1 1451    2
1.000000+0 0.000000+0           0          0         12          6  1 1451    3
0.000000+0 0.000000+0           0          0         32          2  1 1451    4
H(H2O)     LEIP LAB   EVAL-OCT18   C. Manring, Y. Zhu, D. Antony,    1 1451    5
                                                    A.I. Hawari      1 1451    6
                      DIST-                                          1 1451    7
----ENDF/B-VIII.1     MATERIAL  1                                    1 1451    8
-----THERMAL NEUTRON SCATTERING DATA                                 1 1451    9
------ENDF-6 FORMAT                                                 1 1451   10
                                                                     1 1451   11
Temperatures = 283, 293, 300, 323, 350, 373, 400, 423, 450,          1 1451   12
               473, 500, 523, 550, 573, 600, 623, 650 K              1 1451   13
                                                                     1 1451   14
Background                                                           1 1451   15
----------                                                           1 1451   16
          NOTE: THIS LIBRARY IS BETA VERSION: 1                      1 1451   17
Produced/Compatible with the stock NJOY16                            1 1451   18
                                                                     1 1451   19
This library was produced by the Low Energy Interaction Physics      1 1451   20
(LEIP) group at North Carolina State University. The thermal         1 1451   21
scattering law data for hydrogen in H2O were developed using the     1 1451   22
molecular dynamics (MD) method [1]. There is no File 7 MT = 2,       1 1451   23
i.e. coherent elastic cross sections. 17 temperatures are            1 1451   24
available in this library. The LEAPR module from the NJOY 2016       1 1451   25
code system was used to produce File 7 MT = 4 data for H in H2O.     1 1451   26
By convention, MAT = 1 and ZA=1001 are used for H in H2O.            1 1451   27
                                                                     1 1451   28
                                                                     1 1451   29
References                                                           1 1451   30
----------                                                           1 1451   31
                                                                     1 1451   32
1. A.I. Hawari, "Modern Techniques in Inelastic Thermal Neutron      1 1451   33
   Scattering Analysis," Nuclear Data Sheets 118 (2014) 172.         1 1451   34
                                                                     1 1451   35
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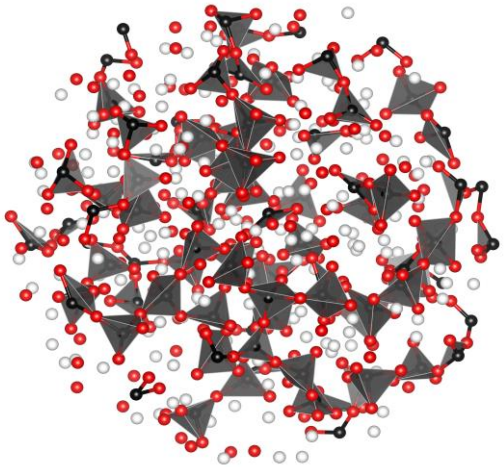
Liquid FLiBe – FY 2019

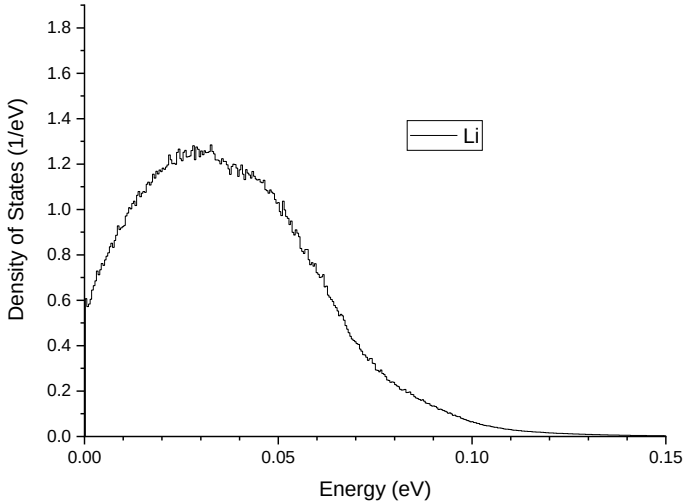


- Eutectic with a mixture of 2:1 ratio of LiF and BeF2
- Melting Point: 732K Boiling Point:1703K
- DFT and MD analysis (with QM corrections)
- TSL evaluation between 750K and 1500K

Born-Mayer potential

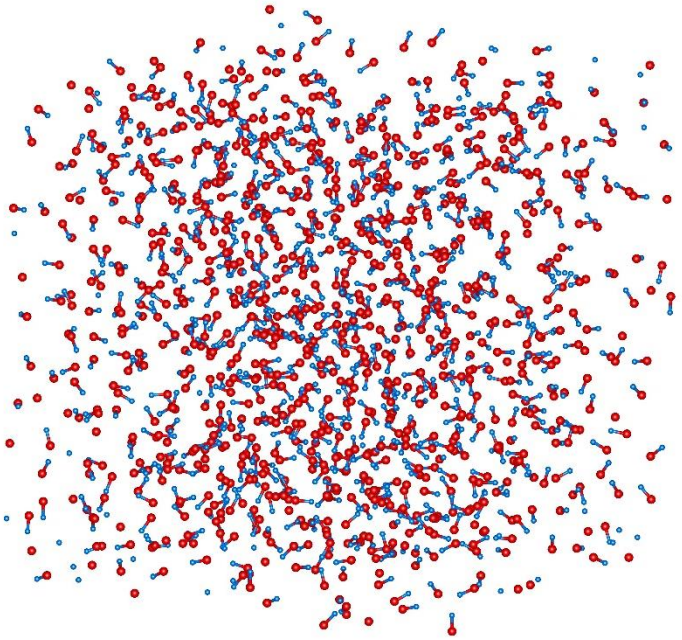
$$U_{i,j}(r_{i,j}) = U_1 + U_2 + U_3 + U_4$$

$$U_1 = \frac{Z_i Z_j e^2}{r_{i,j}}, U_2 = -\frac{c_i c_j}{r_{i,j}^{\,6}}, U_3 = \frac{D}{r_{i,j}^{\,8}}, U_4 = b_{i,j}\left(1 + \frac{Z_i}{N_i} + \frac{Z_j}{N_j}\right)\exp\left(\frac{r_i + r_j - r_{i,j}}{\rho}\right)$$



Hydrofluoric Acid

- Strong hydrogen bonding
- Unique molecular structure dynamics



Example CMD Potential:

Inter-

LJ + 3 pt. chg.

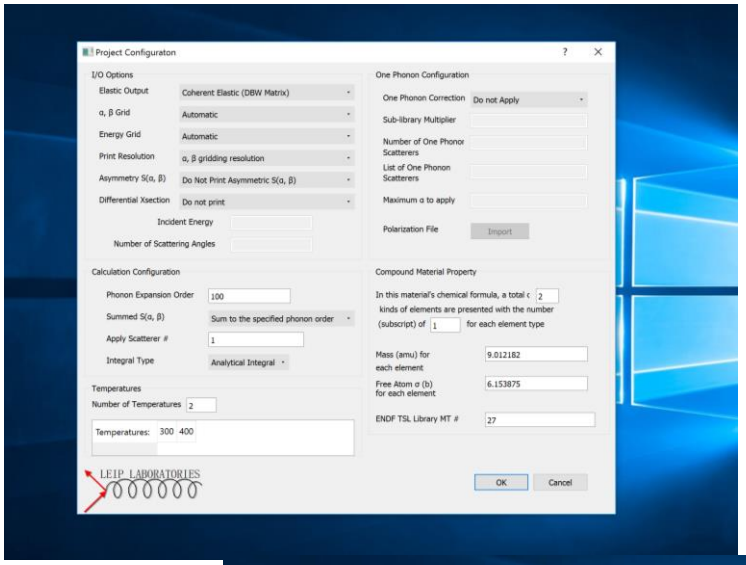
$$V(r) = A\left[\left(\frac{B}{r}\right)^{12} - \left(\frac{B}{r}\right)^{6}\right] + \cdots$$

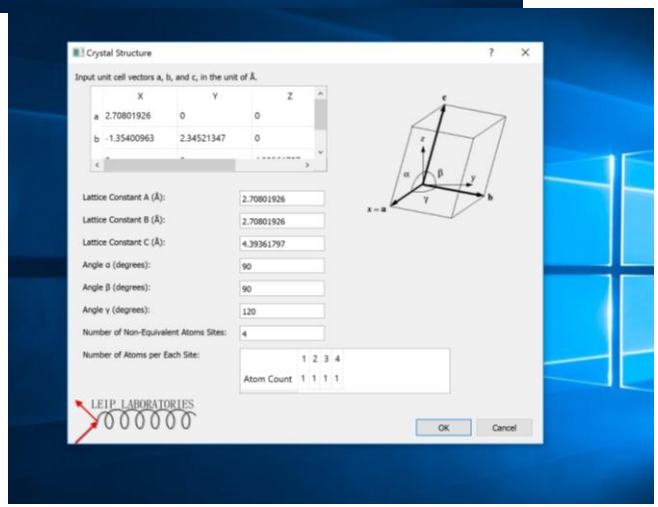
Intra-

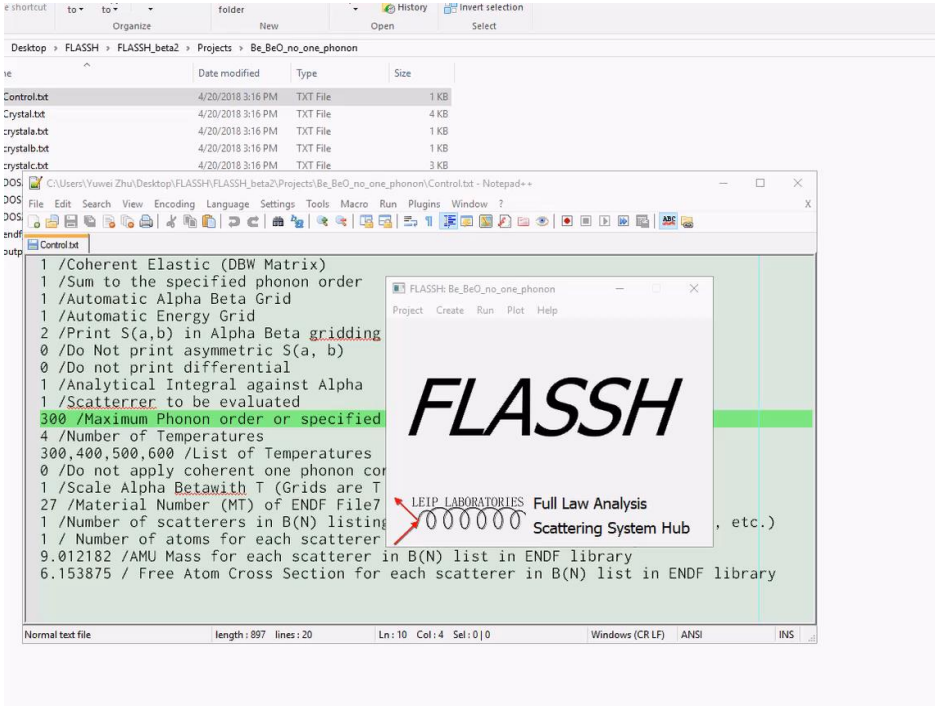
Perturbed Morse Osc.

$$V(r) = C\{exp[-D(r - r_0)] - 1\}^2 + E_r$$

FLASSH Code


Project Configuraton
I/O Options
Elastic Output
Coherent Elastic (DBW Matrix)
α, β Grid
Automatic
Energy Grid
Automatic
Print Resolution
α, β gridding resolution
Asymmetry S(α, β)
Do Not Print Asymmetric S(α, β)
Differential Xsection
Do not print
Incident Energy
Number of Scattering Angles
One Phonon Configuration
One Phonon Correction
Do not Apply
Sub-library Multiplier
Number of One Phonon Scatterers
List of One Phonon Scatterers
Maximum α to apply
Polarization File
Import
Calculation Configuration
Phonon Expansion Order
100
Summed S(α, β)
Sum to the specified phonon order
Apply Scatterer #
1
Integral Type
Analytical Integral
Temperatures
Number of Temperatures
2
Temperatures:
300 400
Compound Material Property
In this material's chemical formula, a total of
2
kinds of elements are presented with the number
(subscript) of
1
for each element type
Mass (amu) for each element
9.012182
Free Atom σ (b) for each element
6.153875
ENDF TSL Library MT #
27
LEIP LABORATORIES
OK
Cancel


Crystal Structure
Input unit cell vectors a, b, and c, in the unit of Å.
X
Y
Z
a
2.70801926
0
0
b
-1.35400963
2.34521347
0
Lattice Constant A (Å):
2.70801926
Lattice Constant B (Å):
2.70801926
Lattice Constant C (Å):
4.39361797
Angle α (degrees):
90
Angle β (degrees):
90
Angle γ (degrees):
120
Number of Non-Equivalent Atoms Sites:
4
Number of Atoms per Each Site:
1 2 3 4
Atom Count
1 1 1 1
LEIP LABORATORIES
OK
Cancel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Type
Size
Control.txt
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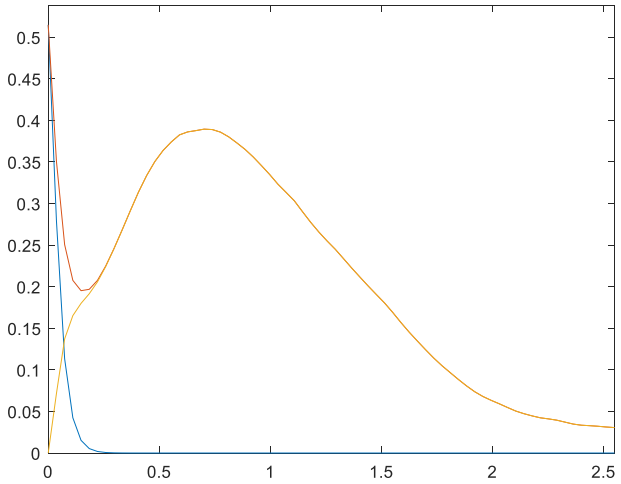
TXT File
1 KB
Crystal.txt
4/20/2018 3:16 PM
TXT File
4 KB
crystala.txt
4/20/2018 3:16 PM
TXT File
1 KB
crystalb.txt
4/20/2018 3:16 PM
TXT File
1 KB
crystalc.txt
4/20/2018 3:16 PM
TXT File
3 KB
C:\Users\Yuwei Zhu\Desktop\FLASSH\FLASSH_beta2\Projects\Be_BeO_no_one_phonon\Control.txt - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?
Control.txt
1 /Coherent Elastic (DBW Matrix)
1 /Sum to the specified phonon order
1 /Automatic Alpha Beta Grid
1 /Automatic Energy Grid
2 /Print S(a,b) in Alpha Beta gridding
0 /Do Not print asymmetric S(a, b)
0 /Do not print differential
1 /Analytical Integral against Alpha
1 /Scatterrer to be evaluated
300 /Maximum Phonon order or specified
4 /Number of Temperatures
300,400,500,600 /List of Temperatures
0 /Do not apply coherent one phonon cor
1 /Scale Alpha Betawith T (Grids are T
27 /Material Number (MT) of ENDF File7
1 /Number of scatterers in B(N) listing
1 / Number of atoms for each scatterer
9.012182 /AMU Mass for each scatterer in B(N) list in ENDF library
6.153875 / Free Atom Cross Section for each scatterer in B(N) list in ENDF library
, etc.)
Normal text file
length : 897 lines : 20
Ln : 10 Col : 4 Sel : 0 | 0
Windows (CR LF)
ANSI
INS
FLASSH: Be_BeO_no_one_phonon
Project Create Run Plot Help
FLASSH
LEIP LABORATORIES
Full Law Analysis
Scattering System Hub

FLASSH Code Features

	NJOY	*FLASSH*
Coherent Inelastic	☐	☑
Remove Incoherent Approximation	☐	☑
Remove Short Collision Time (SCT) Approximation	☐	☑
Integral against alpha differential cross section	Numerical	Default: Analytical Optional: Numerical
a, B Gridding	User input	Default: Automatic grid Optional: User input
Parallel Computing	☐	☑ Using OpenMP
Graphite User Interface	☐	☑
Syntax and Error Checking	☐	☑
Coherent Elastic Calculation		
Supported Structure	Hexagonal, FCC, BCC	Any crystal structure
Supported Materials	Graphite, Beryllium, Beryllium Oxide, Aluminum, Lead, Iron	Any material
Compound Materials	2 elements with ratio 1:1	Any number of elements with any ratio
Remove Cubic Approximation	☐	☑
Remove Atom Site Approximation	☐	☑
Coherent Elastic Scattering Cross Section	Over Ewald Sphere	On every reciprocal lattice point
Need to modify source code if calculating other materials	**Yes**	**No**

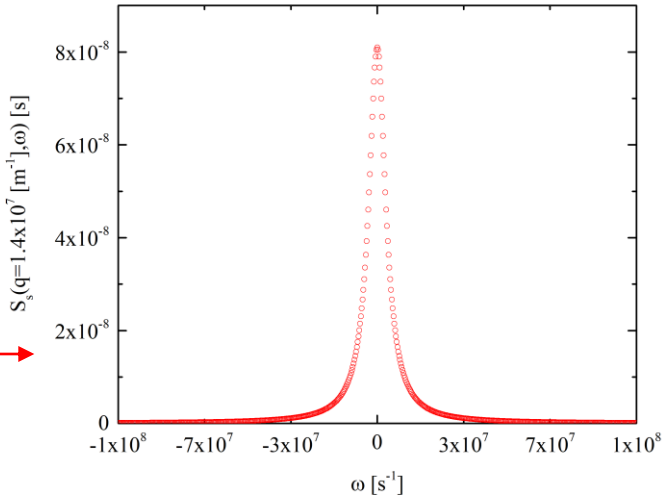
Liquid Physics in *FLASSH*

- **Separation** of the diffusive DOS from the continuous (solid) DOS in LEAPR



- **Convolution** of the solid and liquid TSL components

$$S_{total}(\alpha,\beta) = \left(S_{diff.}(\alpha,\beta) * S_{cont.}(\alpha,\beta)\right)(\beta)$$



Liquid Physics in *FLASSH*

Construct fine beta grid (for convolution):

- Call **convolve_grid** subroutine to determine appropriate resolution and lower/upper beta limits

Build liquid TSL model over the new beta grid:

- Call liquid model function (e.g., **lang** for Langevin)
  - Call **besk1** (Bessel) function if necessary

Interpolate solid TSL onto new beta grid:

- Call **interp_grid** subroutine to interpolate values for every convolution 'window'

Convolve the liquid and solid components:

- Call **convolve** subroutine to perform the convolution

Construct total TSL:

- Add in extra DW term

Output results:

- Write TSL components to various files

Doppler Broadening

- Free Gas
  - Assumes a Maxwellian velocity distribution

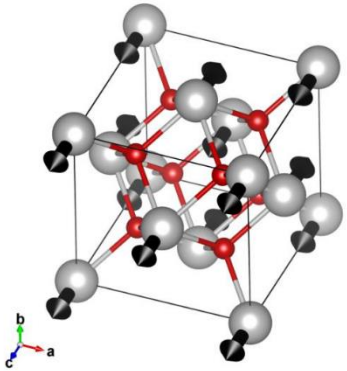
$$\sigma^{FG}(E) = \int_0^\infty dE'\, S^{FG}(E',E)\sigma(E'),\;\; S^{FG}(E',E) = \frac{1}{\Delta\sqrt{\pi}}\sqrt{\frac{E'}{E}}\exp\left[\frac{-(E'-E)^2}{\Delta^2}\right]$$

- Crystal Lattice
  - Compound nucleus effects separated from lattice effects
  - Transition probability
  - Self Scattering Law
    - Identical to that used in thermal scattering
    - Describes the energy-momentum phase space of a material

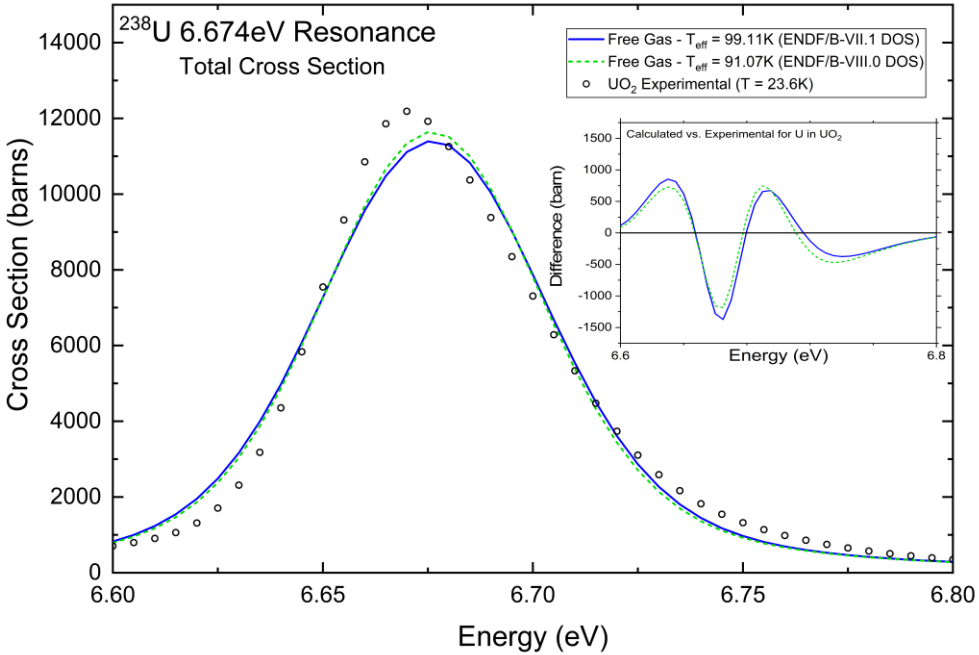
$$\sigma(E) = \frac{\sigma_0\Gamma^2}{4}\int_{-\infty}^{\infty} d\beta\, \frac{S_s(\alpha,\beta)}{(E - E_0 - \beta k_B T)^2 + (\Gamma/2)^2}$$

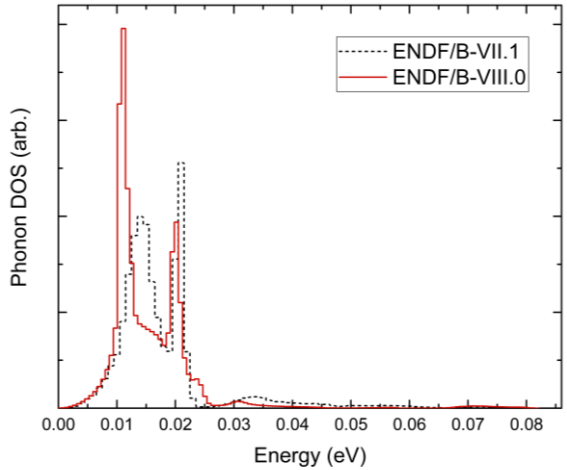
Doppler Broadening

- *Ab initio* lattice dynamics
  - Predictive density of states (DOS)
  - Current DOS implemented in the ENDF/B-VIII.0 cross section library for U in UO_2



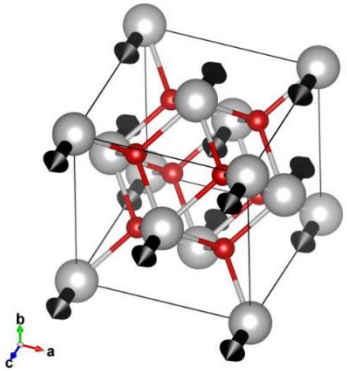
- Fluorite Structure
- 2x2x2 supercell
- GGA-PBE+U





Doppler Broadening

- *Ab initio* lattice dynamics
  - Predictive density of states (DOS)
  - Current DOS implemented in the ENDF/B-VIII.0 cross section library for U in UO_2



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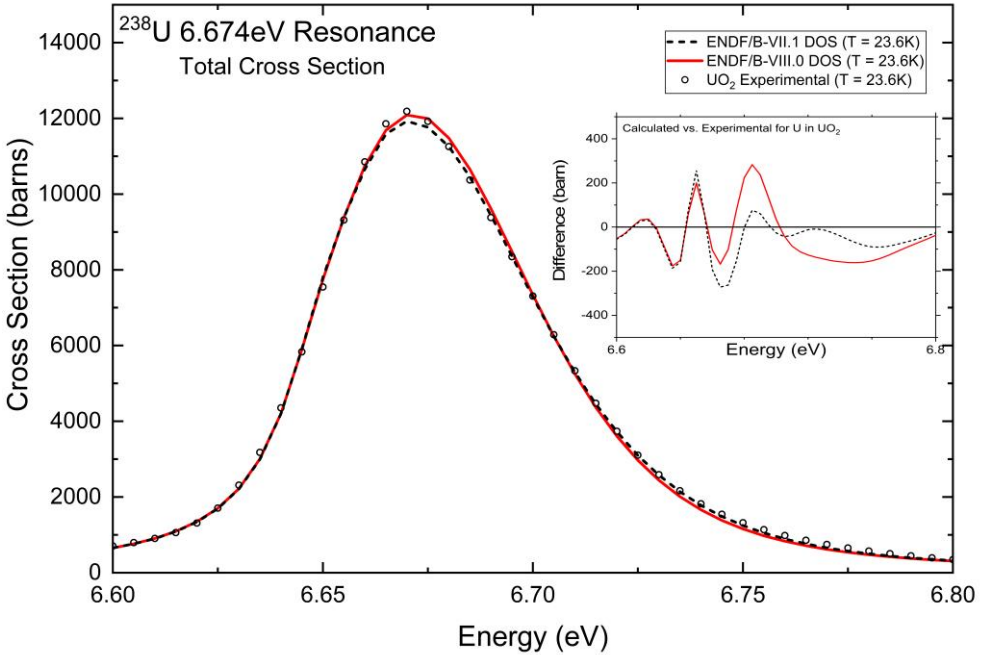
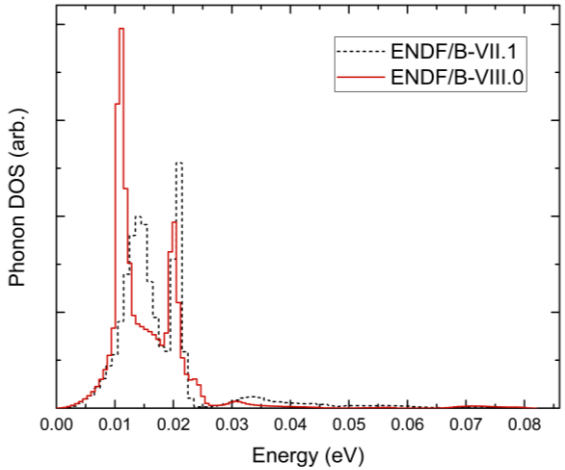




FLASSH Generalized TSL

$$S_s(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar}\int e^{-i\omega t} e^{\langle U^2\rangle + \langle UV_0\rangle} dt = \mathrm{e}^{-2W}\sum_{n=0}^{\infty}\frac{(2W)^n}{n!}G_n$$

Full Equation

$$\sum_s (\vec{\kappa}\cdot\vec{e}_s)^2 = \frac{1}{3}k^2$$

Cubic Approximation

$$G_1(\omega) = \frac{1}{\gamma(0)}\frac{1}{N}\frac{\hbar}{k_B T}\sum_s \frac{\left|\vec{e}_\kappa \square \vec{e}_s\right|^2}{2\beta\sinh(\beta/2)} e^{-\beta/2}$$

$$2W = \frac{\hbar}{2MN}\sum_s \frac{\left|\vec{\kappa}\cdot\vec{e}_s\right|^2}{\omega_s}\coth\left(\frac{\hbar\omega_s}{2k_B T}\right)$$

- Function of the polarization vector and dispersion relations

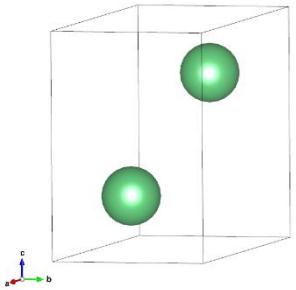
$$G_1(\omega) = \frac{1}{\lambda}\frac{\rho(\beta)}{2\beta\sinh(\beta/2)} e^{-\beta/2}$$

$$2W = \frac{\hbar k^2}{2M}\int_0^{\omega_m}\frac{\rho(\omega)}{\omega}\coth\left(\frac{\hbar\omega_s}{2k_B T}\right)d\omega$$

- Function of the density of states ρ(ω)

FLASSH Generalized TSL

- Beryllium Metal
  - HCP (P63/mmc)
  - *Ab initio* lattice dynamics
  - 4x4x3 Supercell



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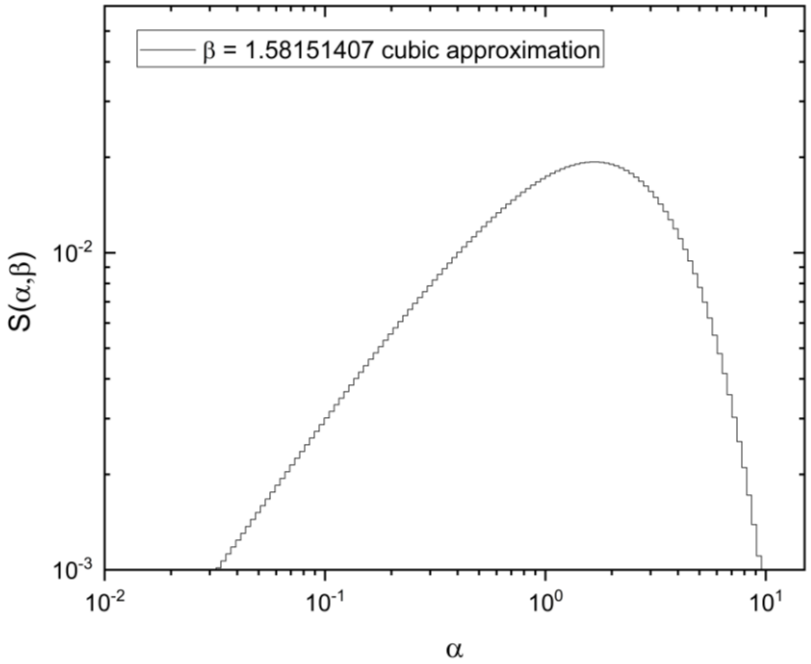
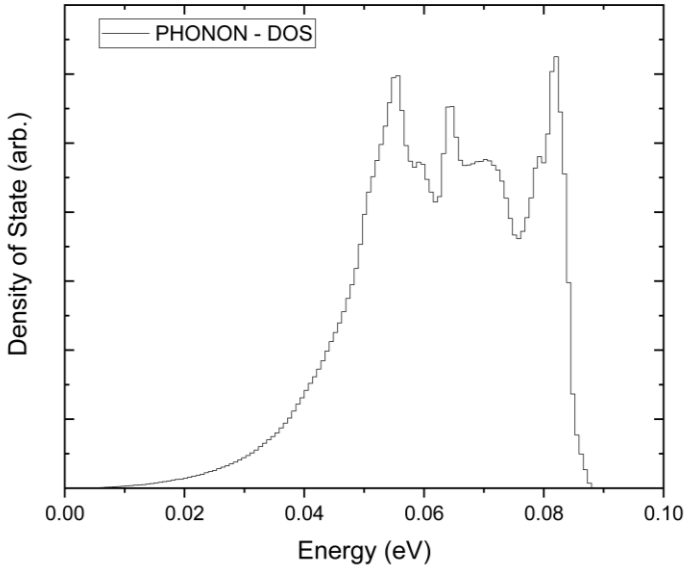
0	5.49E-3	0
0	0	5.49E-3

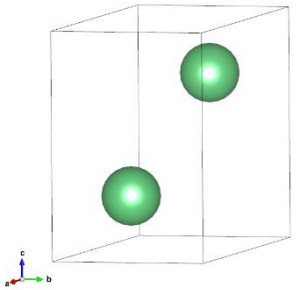
Exact Debye-Waller Matrix ($Å^2$)





FLASSH Generalized TSL

- Beryllium Metal
  - HCP (P63/mmc)
  - *Ab initio* lattice dynamics
  - 4x4x3 Supercell



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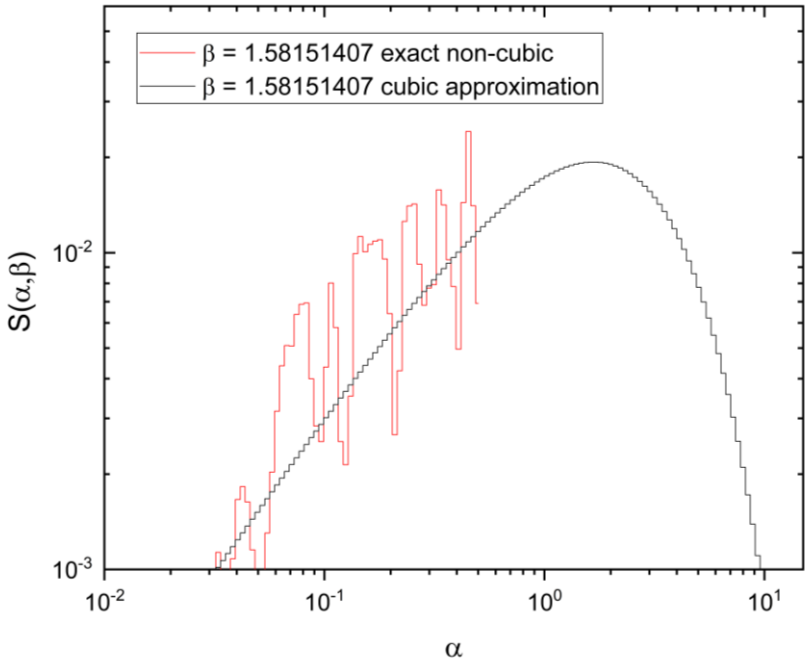
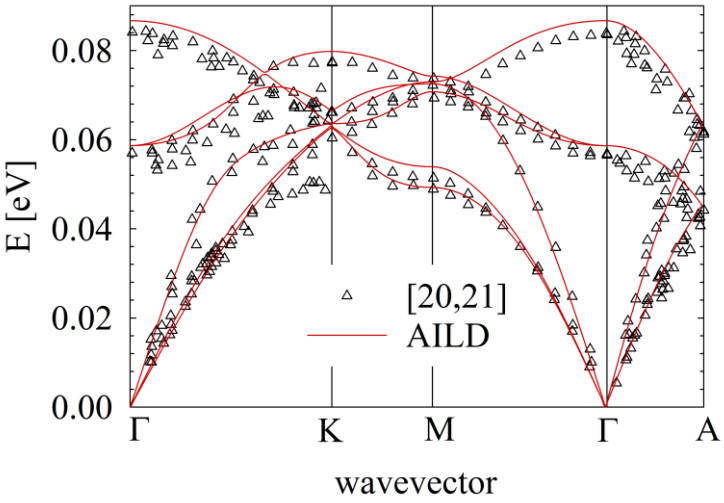
-1.58E-5	5.74E-3	-5.18E-7
1.01E-6	-5.18E-7	5.02E-3

Exact Debye-Waller Matrix (Å²)





FUDGE/GNDS

- Ongoing collaboration with LLNL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                                                  A.I. Hawari
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----ENDF/B-VIII.1     MATERIAL  1
-----THERMAL NEUTRON SCATTERING DATA
------ENDF-6 FORMAT

 Temperatures = 283 K

 Background
 ----------
          NOTE: THIS LIBRARY IS BETA VERSION: 1

 This library was produced by the Low Energy Interaction Physics
 (LEIP) group at North Carolina State University. The thermal
 scattering law data for hydrogen in H2O were developed using the
 molecular dynamics (MD) method [1]. There is no File 7 MT = 2,
 i.e. coherent elastic cross sections. One temperature is
 available in this library. The LEAPR module from the NJOY 2016
 code system was used to produce File 7 MT = 4 data for H in H2O.
 By convention, MAT = 1 and ZA=1001 are used for H in H2O.


 References
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 1. A.I. Hawari, "Modern Techniques in Inelastic Thermal Neutron
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Summary

- FY 2018
  - 10 new TSL evaluations contributed to ENDF/B-VIII.0
  - 5 first-of-a-kind evaluations
- FY 2019
  - 4 new TSL evaluations
  - 3 first-of-a-kind evaluations
- Modern predictive methods for thermal neutron cross section calculations based on the use of atomistic simulations
  - Ab initio lattice dynamics
  - Molecular dynamics (ab initio and classical)
    - New materials
    - All states of matter (solid, liquid, gas)
    - Imperfect structure
- *FLASSH* is a new thermal scattering analysis platform that uses a generalized theoretical approach for TSL calculations
  - Removed approximations such as incoherent approximation, cubic approximation, atom site approximation and SCT approximation
- Progress on FY 2019 tasks