



# **Thermal Scattering Law Evaluations and Progress at NCSU**

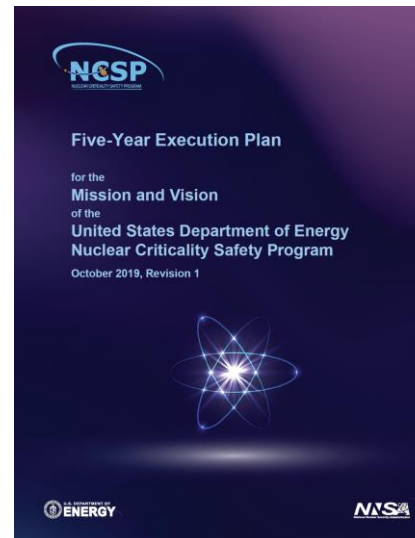
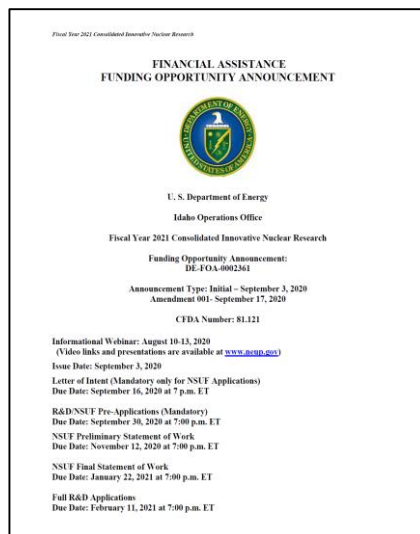
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Laramee, J. Crozier, T. Ahmed**

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Department of Nuclear Engineering  
North Carolina State University  
Raleigh, North Carolina, USA**

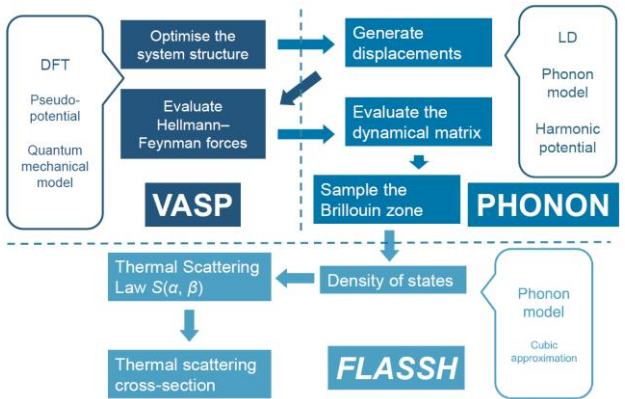
Nuclear Data Week (CSEWG-USNDP-NDAG)  
November 30 – December 4, 2020

# Acknowledgment

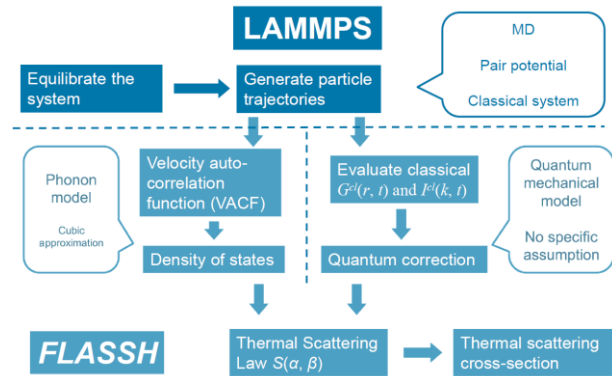
- ❑ DOE NE through the Nuclear Energy University Program (NEUP)
- ❑ NNSA Nuclear Criticality Safety Program (NCSP)
  - in collaboration with LLNL
- ❑ Naval Nuclear Propulsion Program (NNPP)



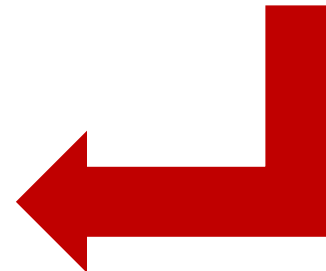
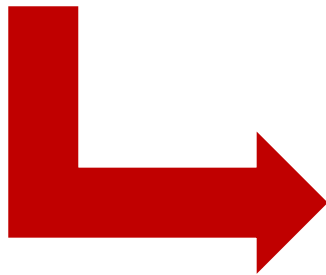
# TSL Methodology



DFT/LD approach



MD approach



Crystal Structure: U\_UN

Material Selection: 12 - U in UN

Parameters [a b c [Å] α β γ [°] (space group)]: 4.85945 4.85945 4.85945 90 90 90 (Fm-3m)

Input unit cell vectors a, b, and c, in the unit of Å.

	X	Y	Z
a	4.85945	0.00000	0.00000
b	0.00000	4.85945	0.00000
c	0.00000	0.00000	4.85945

Number of Non-Equivalent Atoms Sites: 2

DOS Type: Atom site

FLASSH: U\_UN

Project Create Run Help

# FLASSH

Full Law Analysis Scattering System Hub

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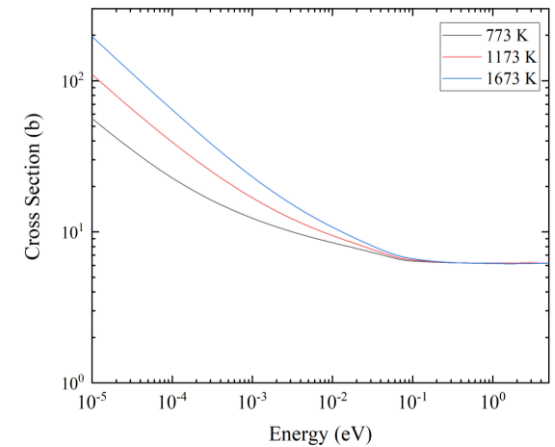
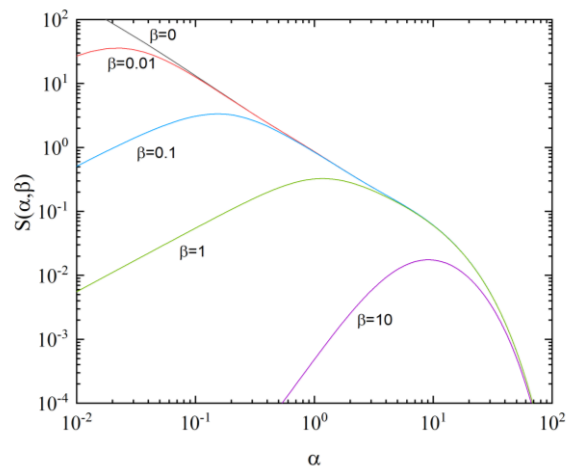
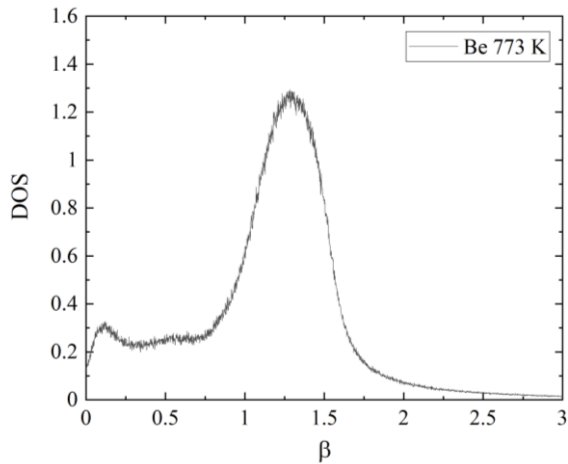
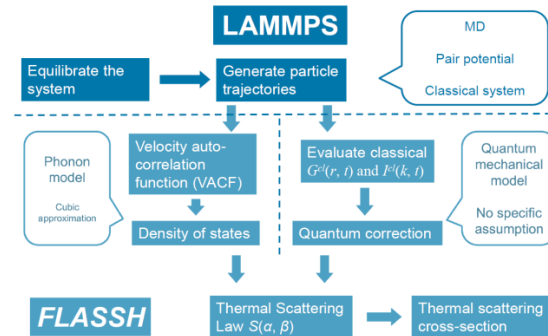
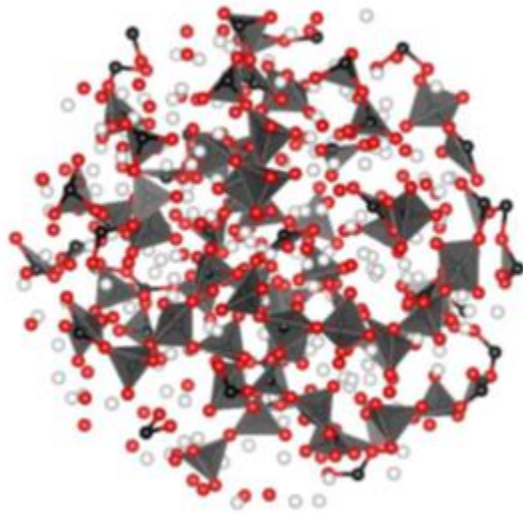
LEIP LABORATORIES

# Contributed TSL Evaluations

Material	Motivation	Theory	Validation
<b>FLiBe (beryllium)</b>	DOE NE Advanced nuclear reactors No TSL data in ENDF/B-VIII.0	MD <i>FLASSH</i>	Ongoing against IRPhEP benchmark
<b>FLiBe (fluorine)</b>			
<b>FLiBe (lithium)</b>			
<b>Liquid hydrogen fluoride (hydrogen)</b>	NCSP applications No TSL data in ENDF/B-VIII.0	MD <i>FLASSH</i>	Ongoing total cross section
<b>Heavy oil (hydrogen)</b>	NCSP/NR applications No TSL data in ENDF/B-VIII.0	MD <i>FLASSH</i>	Ongoing total cross section
<b>Sapphire (Al in Al<sub>2</sub>O<sub>3</sub>)</b>	Neutron science / Research Reactors No TSL data in ENDF/B-VIII.0 (cryogenic temperatures)	DFT/LD <i>FLASSH</i>	Total cross section
<b>Sapphire (O in Al<sub>2</sub>O<sub>3</sub>)</b>			
<b>Polyethylene (hydrogen)</b>	NCSP applications Extended ENDF/B-VIII.0 to cryogenic temperature	MD <i>FLASSH</i>	Total cross section & benchmarks

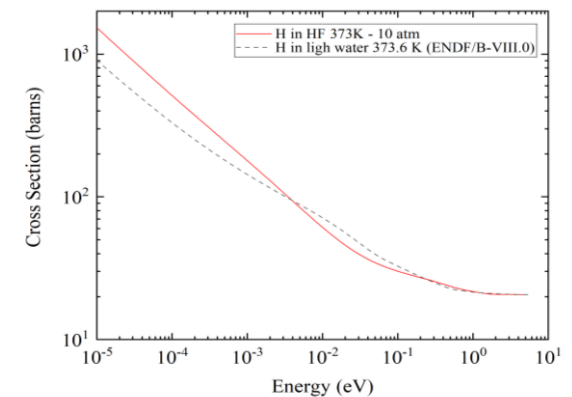
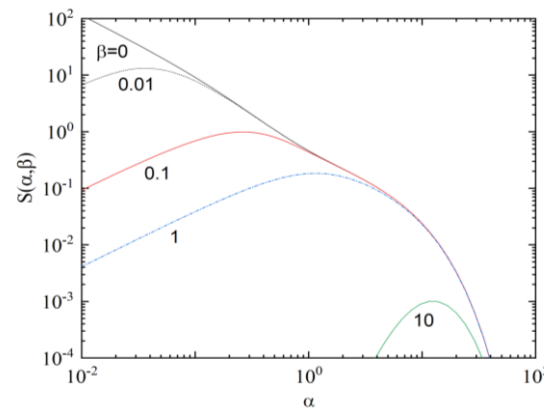
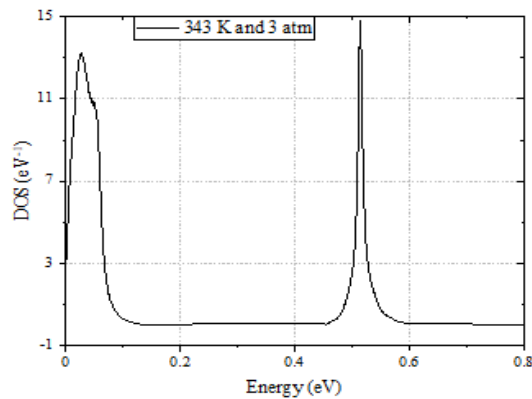
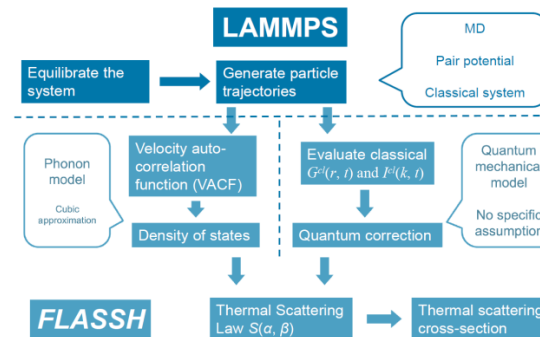
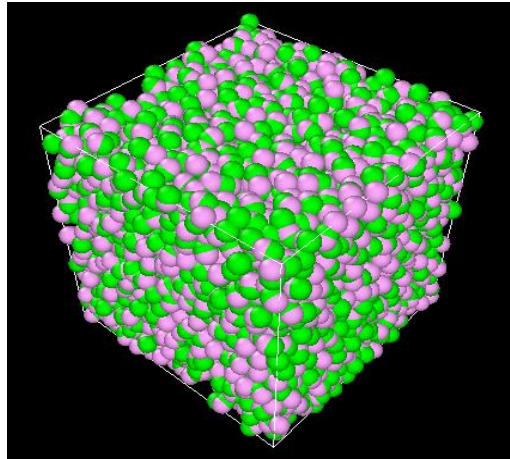
# New to NNDC

## Molten Salt FLiBe Data – DOE NE



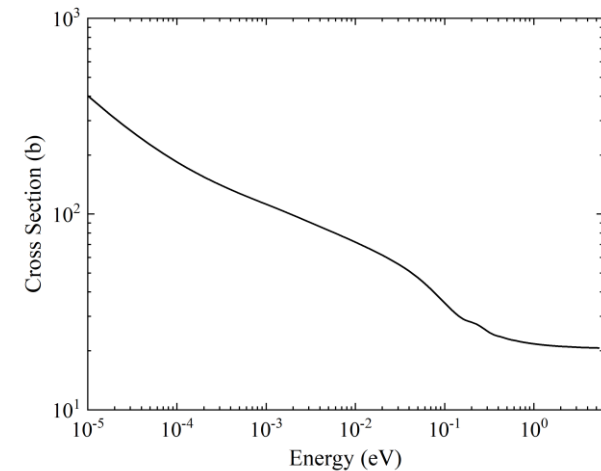
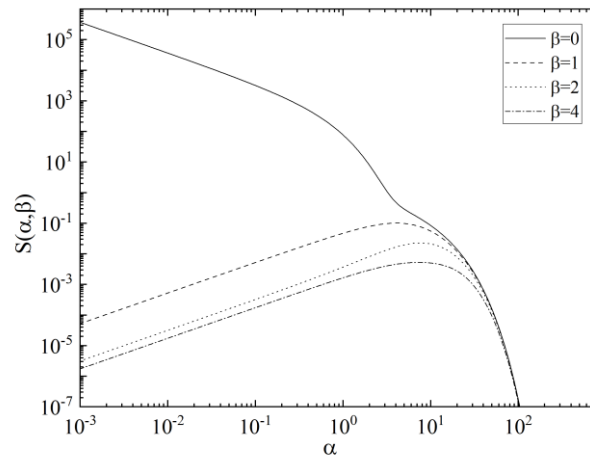
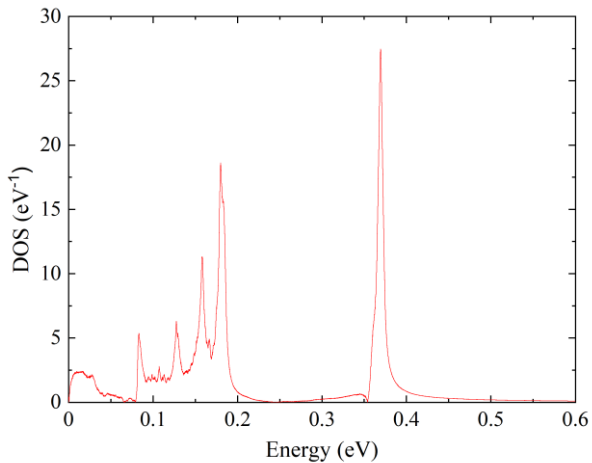
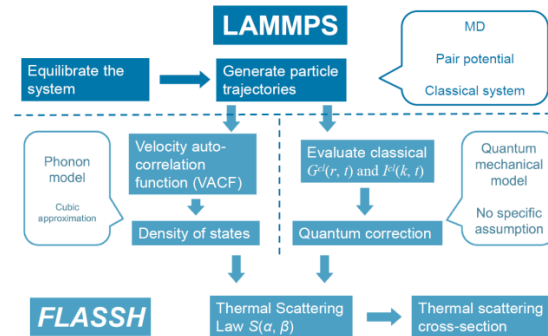
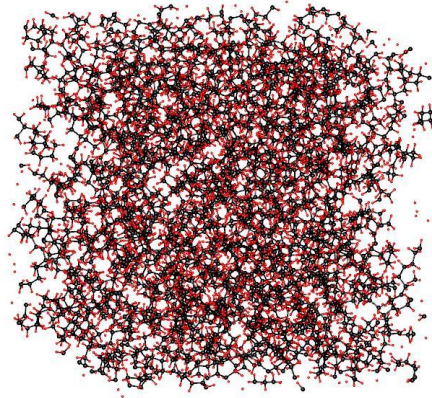
# New to NNDC

## Hydrofluoric Acid Data - NCSP



# New to NNDC

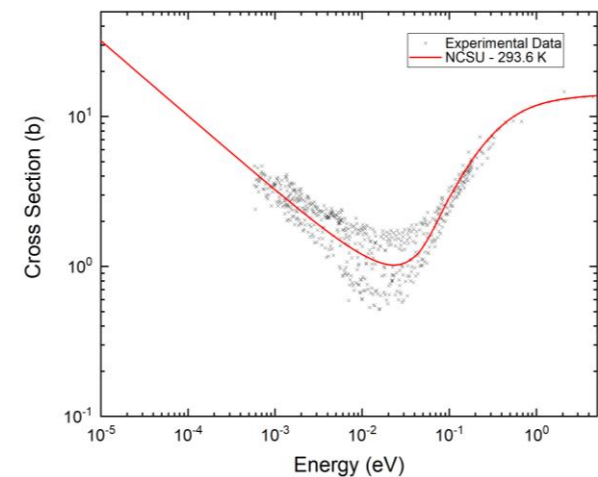
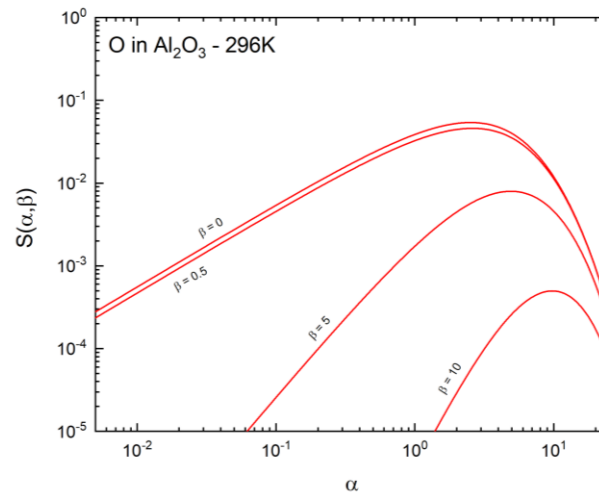
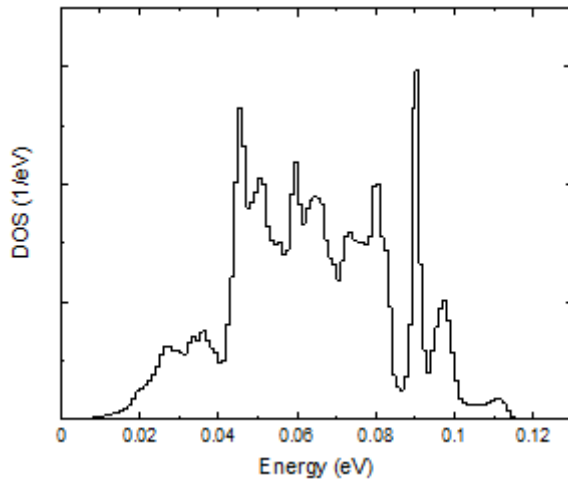
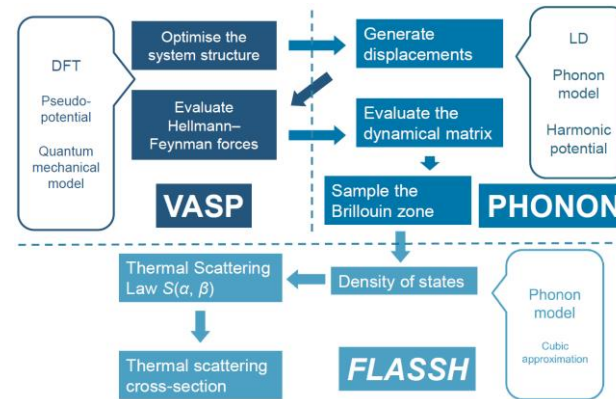
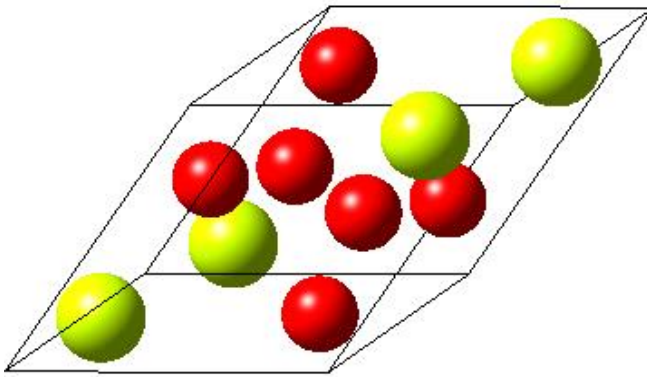
## Heavy Paraffinic Oil Data – NCSP/NR





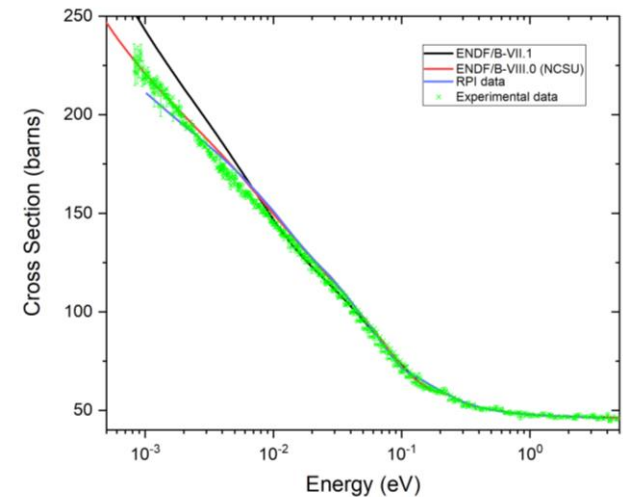
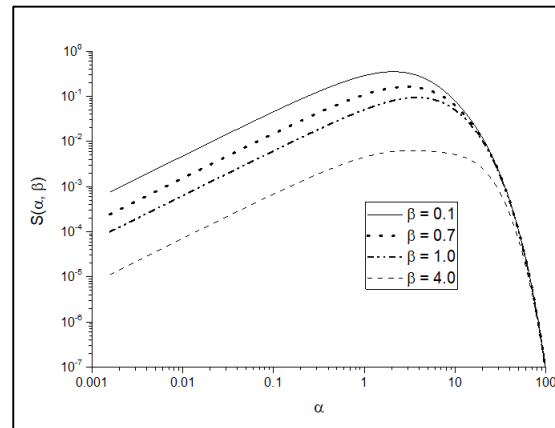
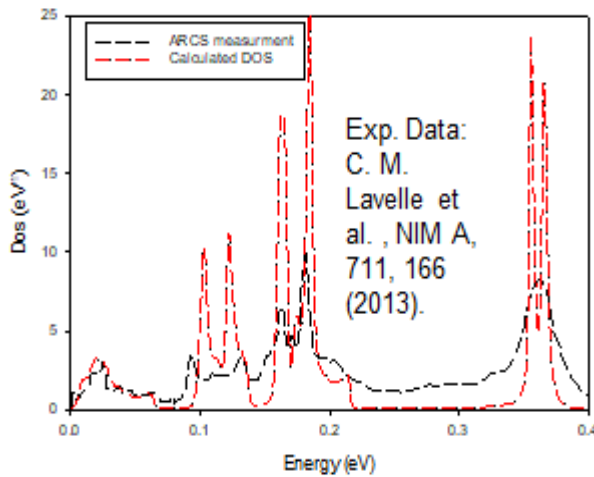
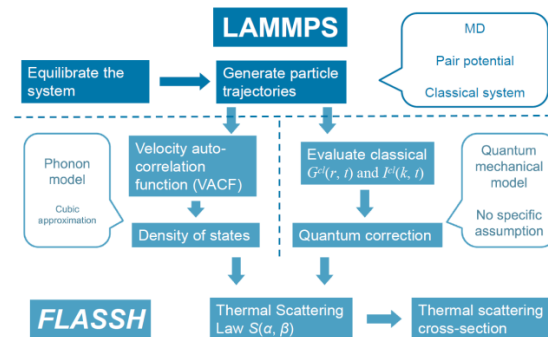
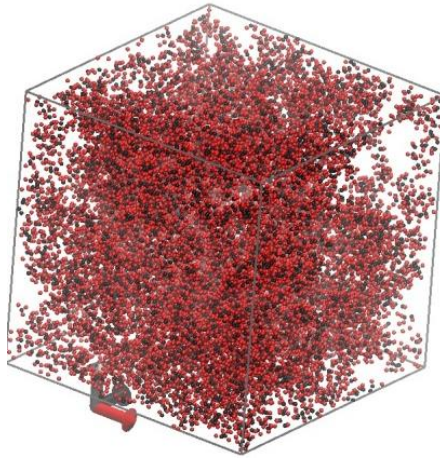
# New to NNDC

## Single Crystal Sapphire Data - RR





# Update to NNDC Polyethylene Data - NCSP



# Summary

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- ❑ 8 new TSL evaluations have been submitted to NNDC
- ❑ All evaluations are performed using the NCSU *FLASSH* code
  - NJOY/LEAPR input files are provided to allow for independent testing
- ❑ Expect more evaluations to be submitted before end of 2020.