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Neutron Thermalization in UN: a Fuel Candidate for LWRs

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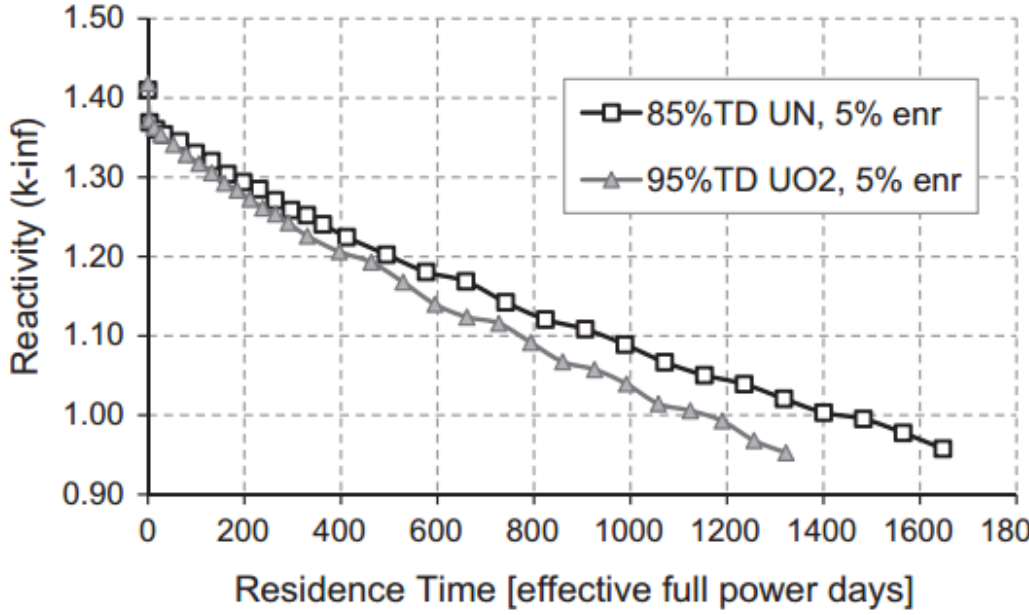
Motivation

To develop **accident tolerant fuel (ATF)** that enhances fuel performance while maintaining compatibility with the existing infrastructure

To date, no thermal neutron scattering cross sections ENDF libraries are available for UN



Feng et al., 2012. J. Nucl. Mater. 427, 30

Objectives

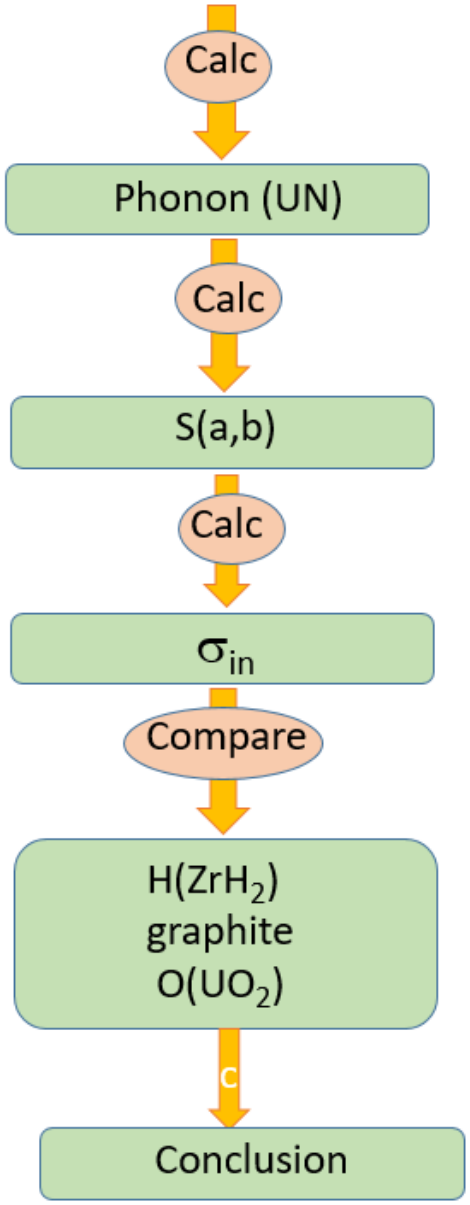
- To study the vibrational properties of UN^{nat} and UN^{15} using *ab initio* lattice dynamics

- To calculate the scattering law at different temperatures

- To calculate the inelastic scattering cross sections of N^{nat}, N^{15} and U in UN at different temperatures

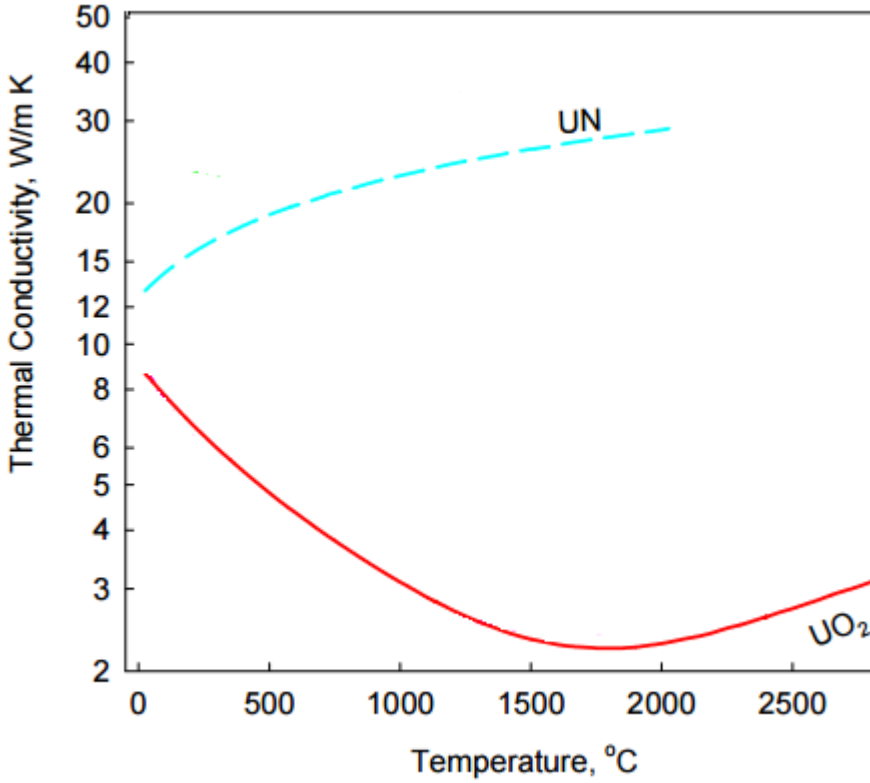
- To compare the inelastic scattering cross sections of N^{15} in UN with those of H in ZrH_2, graphite and O in UO_2.

Outline


Calc
Phonon (UN)
Calc
S(a,b)
Calc
σ_{in}
Compare
H(ZrH_2)
graphite
O(UO_2)
Conclusion

Why UN?

	UN	UO2
Thermal Conductivity	high	Low ???
Uranium Density (g/cm$^{3)}$	13.52	9.65
Thermal Expansion (x 10^{-6} /K) (At 1000 C)	9.2	11.1
Melting Point (K)	3035	3138



Challenges

- UN reacts chemically with water especially at high temperatures
- UN React with nickel (a major component of Alloy -718)

➔ Shielding by ZrO_2 ,U_3Si_2, or U_3Si_5

- N^{14} has high absorption cross section
- N^{14} can transmute into C^{14} ($T_{1/2}$ = 5730 yr)

	N^{14}	N^{15}
s_a (b)	1.91	0.000024

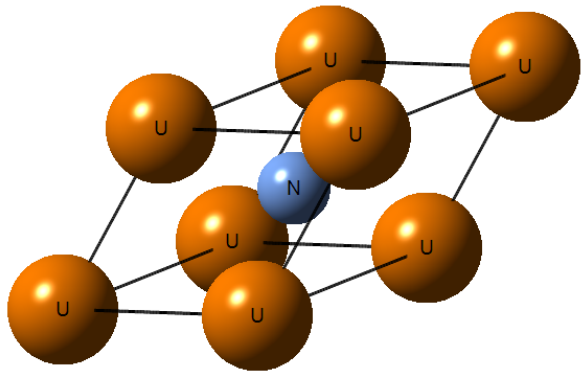
➔ Enriched UN by N^{15} (Recently: can be done economically on a larage scale)

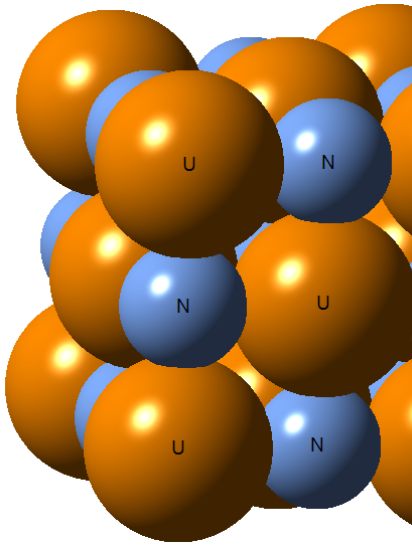
Ab Initio Calculations

UN Crystal Structure

- Rock-Salt structure
- Two atoms per primitive unit cell

  U: (0, 0, 0), O: (1/2, 1/2, 1/2)



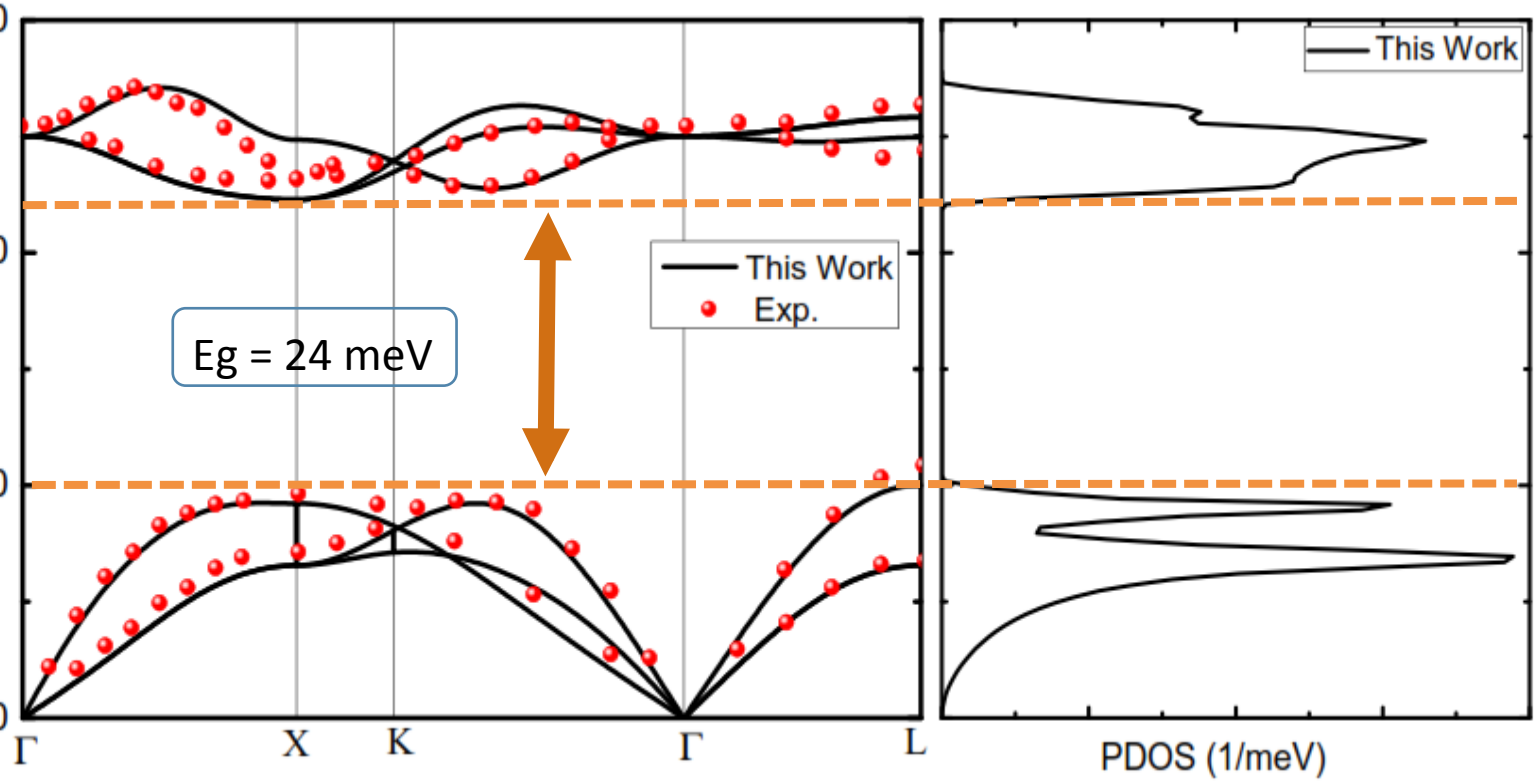


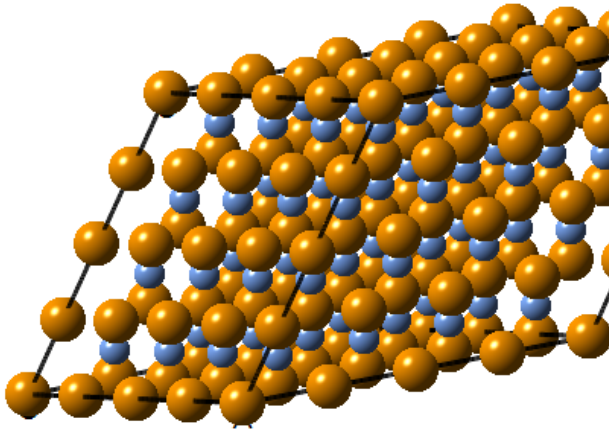
- Structure optimization

	***a* (Å)**	**Ref.**
This Work	4.868	
SP-GGA	4.866	Mei et al., J. Nucl. Mater. 440, 63 (2013)
Exp	4.889	Olsen et al., J. App. Crys. 18, 37 (1985)

- PAW
- VASP code
- SP-GGA
- Ecut = 600 eV
- 8 x8x8 k-mesh

UN^{nat} Phonon Dispersion Relations

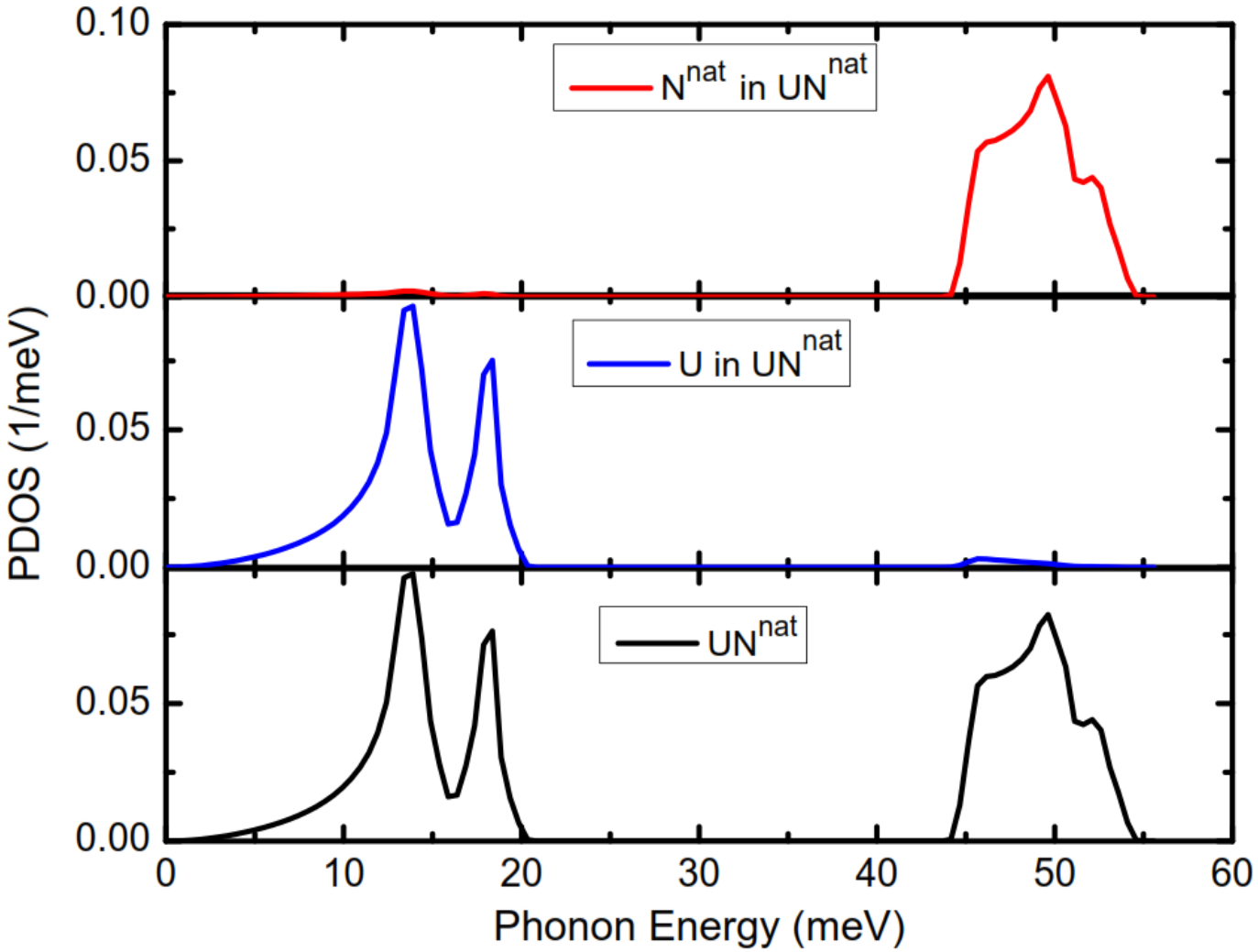




- Phonopy
- VASP
- 4 x 4 x 4 supercell
- 128 atoms
- 2 atomic displacemer
- SP-GGA
- Ecut = 600 eV
- 3 x 3 x 3 k-mesh

	N^{14}	N^{15}	N^{nat}
%	99.63	0.37	100
A (*u*)	14.003074	15.000108	14.006763

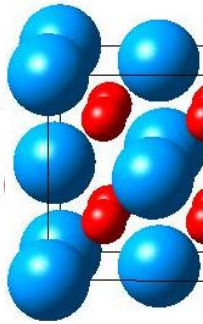
Phonon Density of States (PDOS)

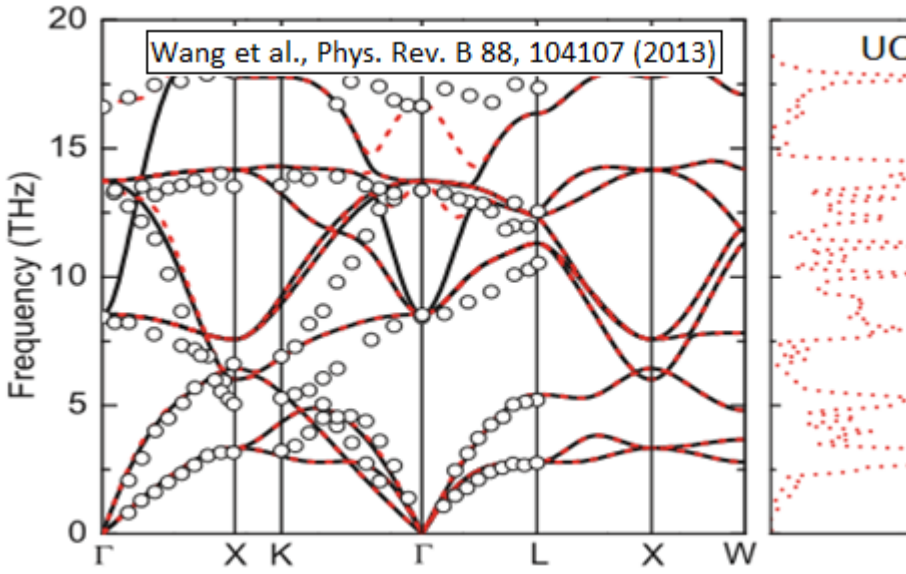


Phonon Density of States (PDOS)

- Phonon energy gap depends on the crystal structure and masses ratio

Structure	Example	Bravis Lattice	Energy Gap
Rock-Salt	MgO, CaO, SrO, BaO	FCC	No
Wurtzite	BeO	Hexagonal	Yes
Rock-Salt	UN	FCC	Yes
Fluorite	UO_2	FCC	No

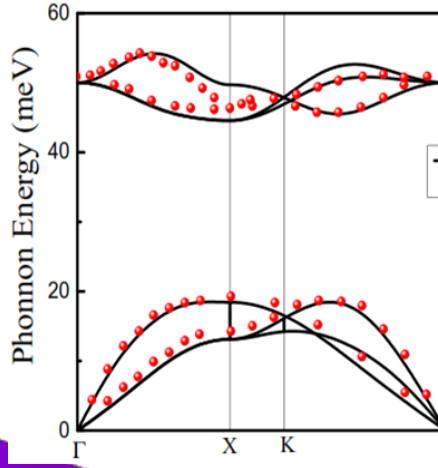


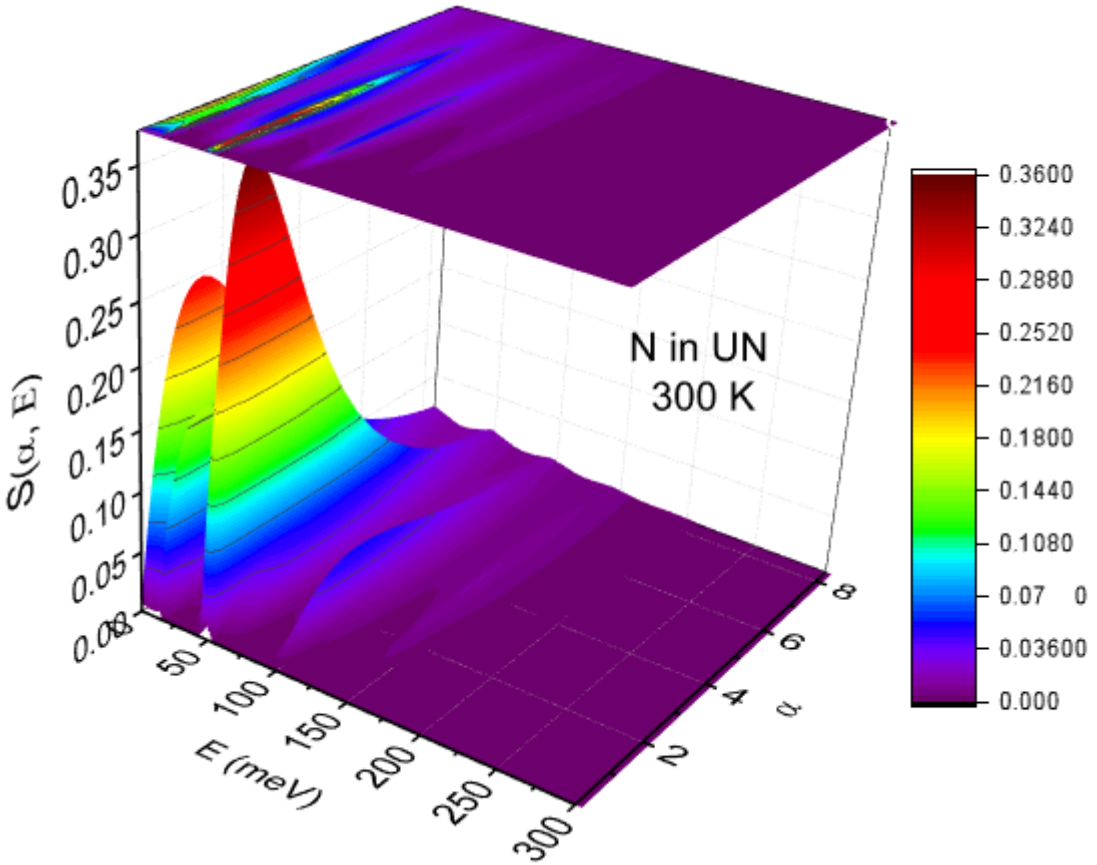


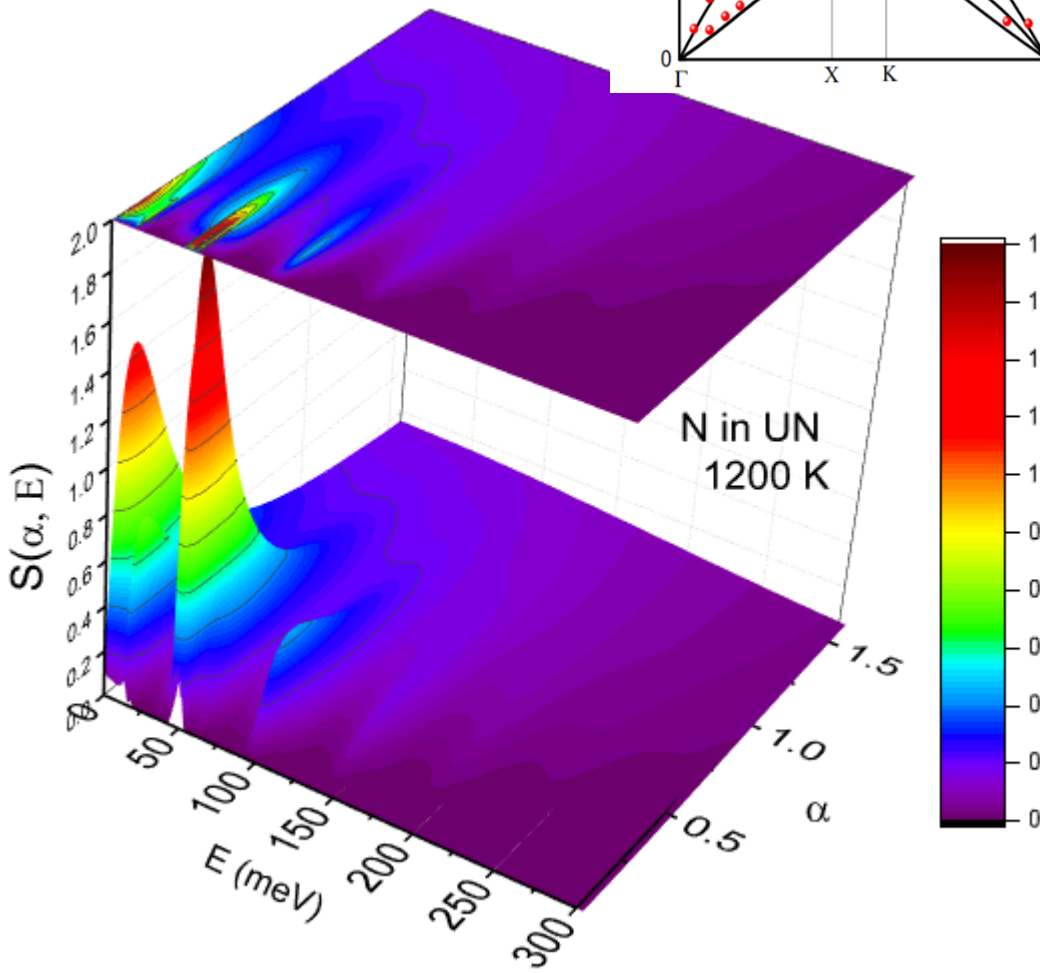
Thermal Neutron Scattering Calculations

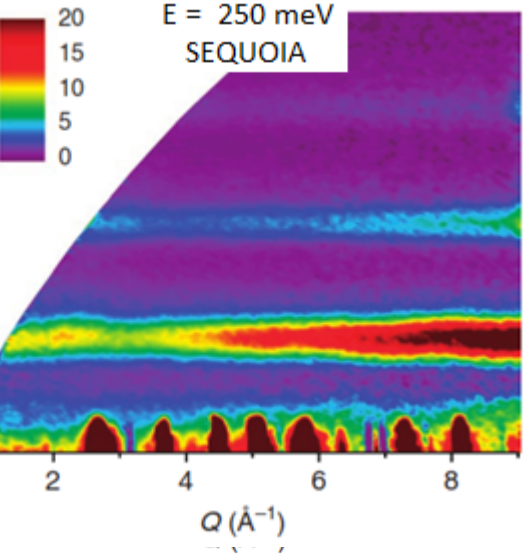
Scattering Law

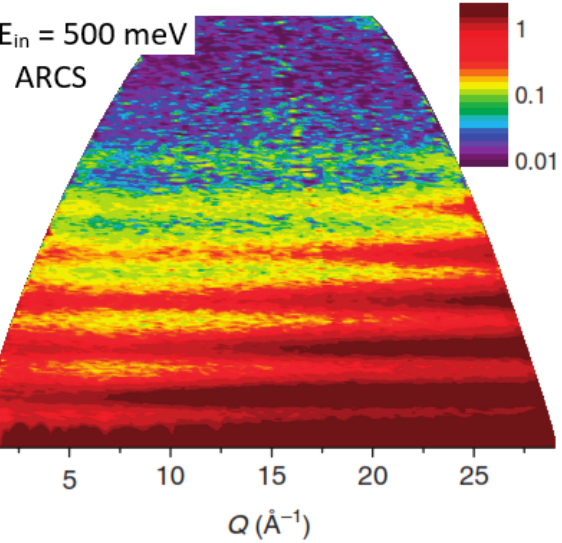
- Simplified
- Equally-spaced and Well-defined
- Extends to very high energies

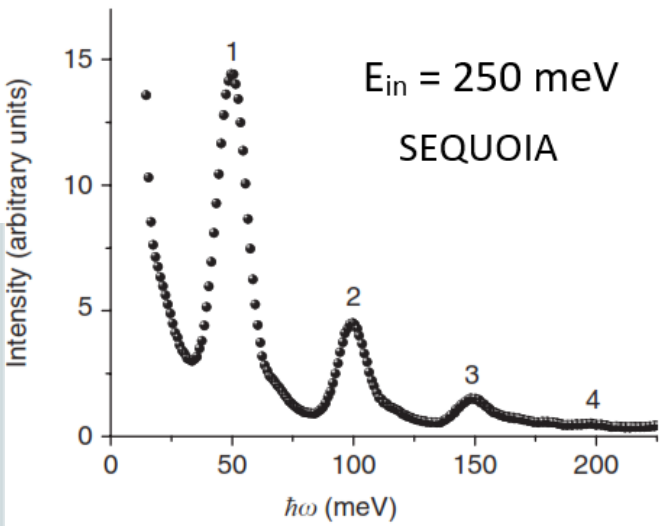


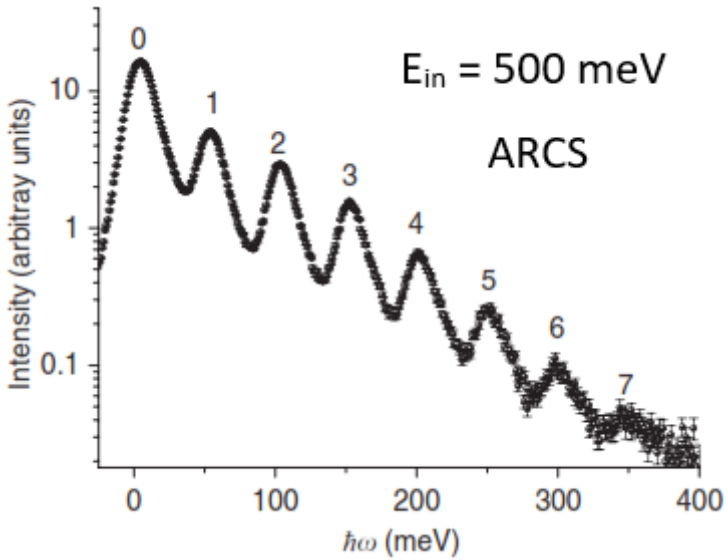


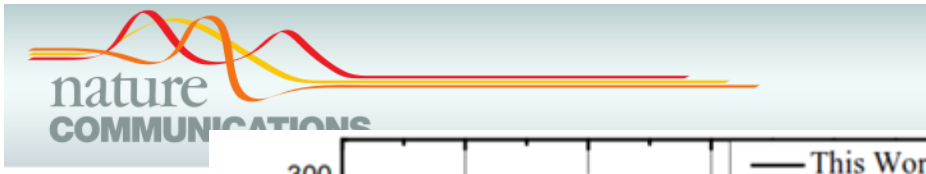












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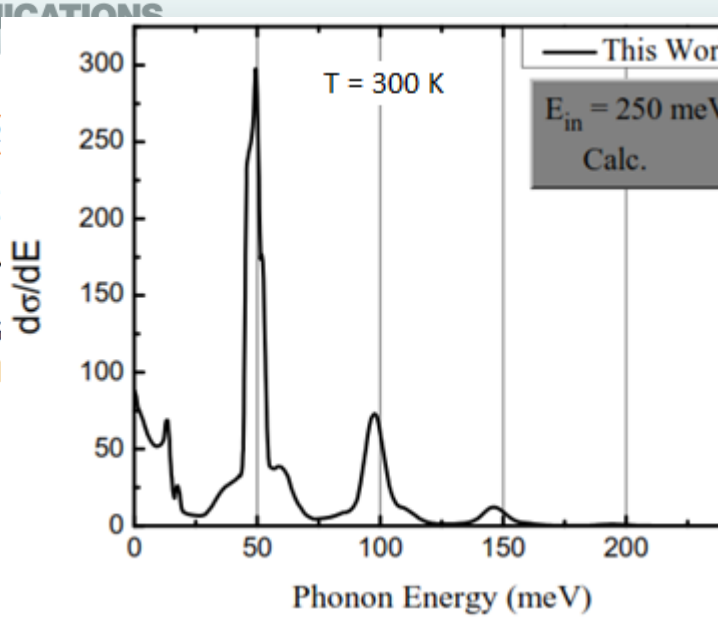
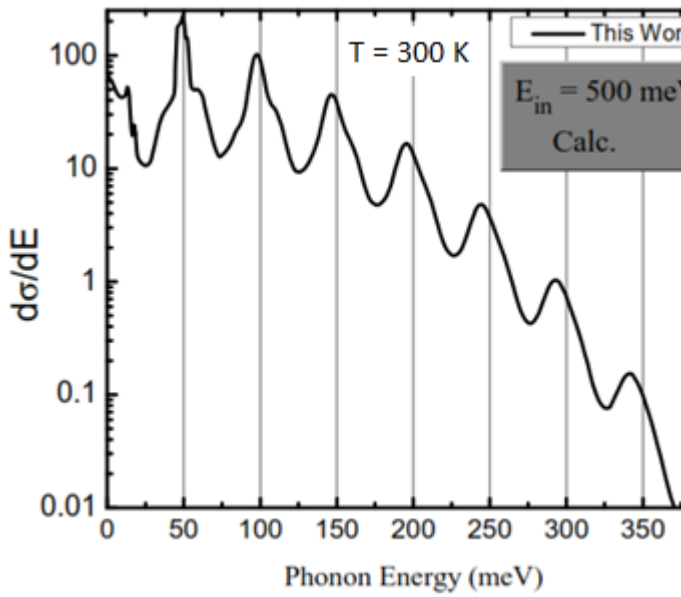
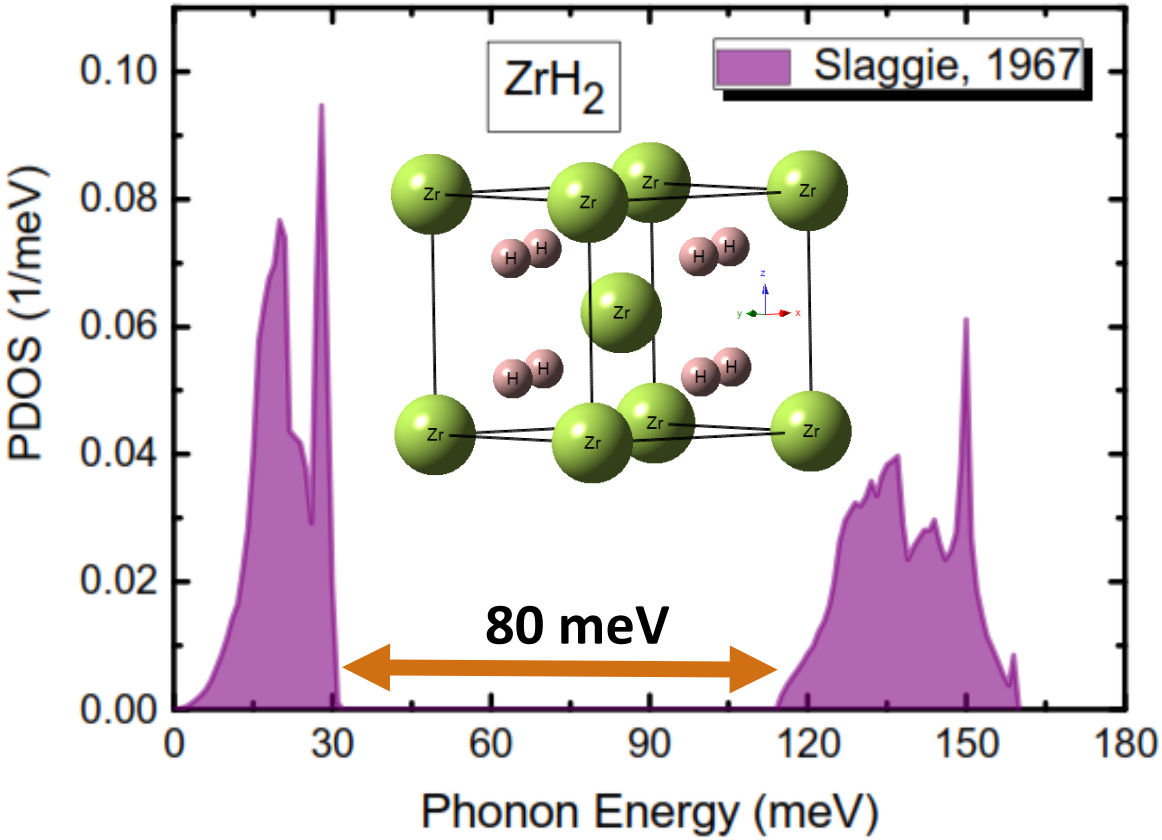


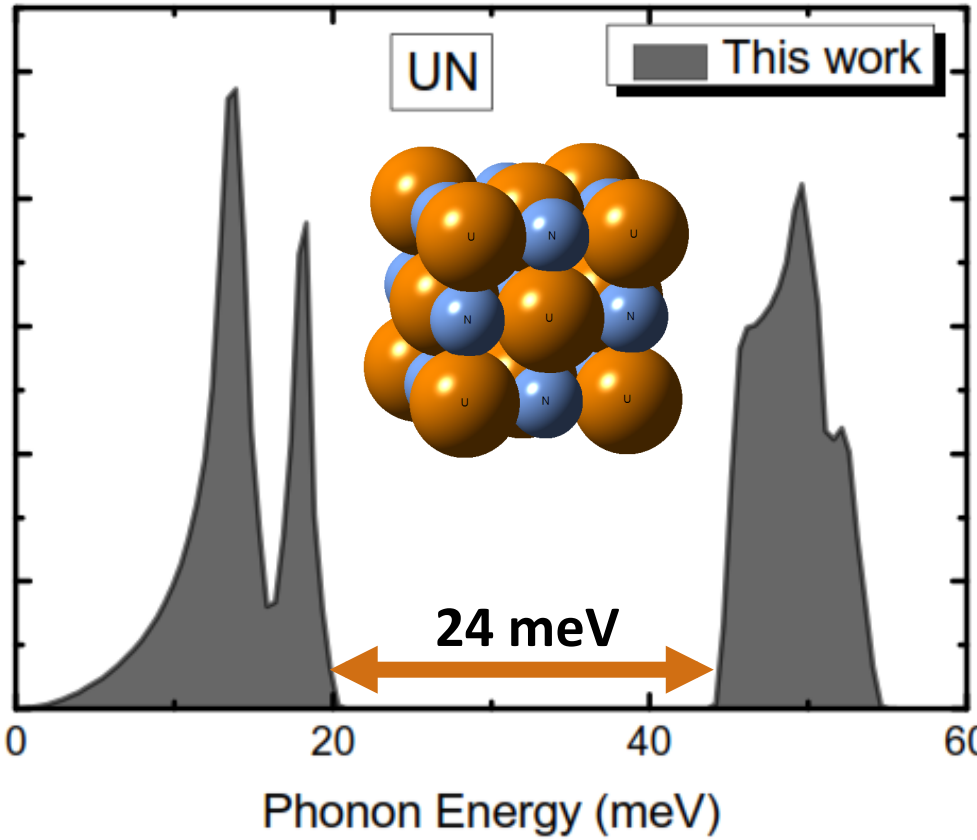


N vs ZrH_2

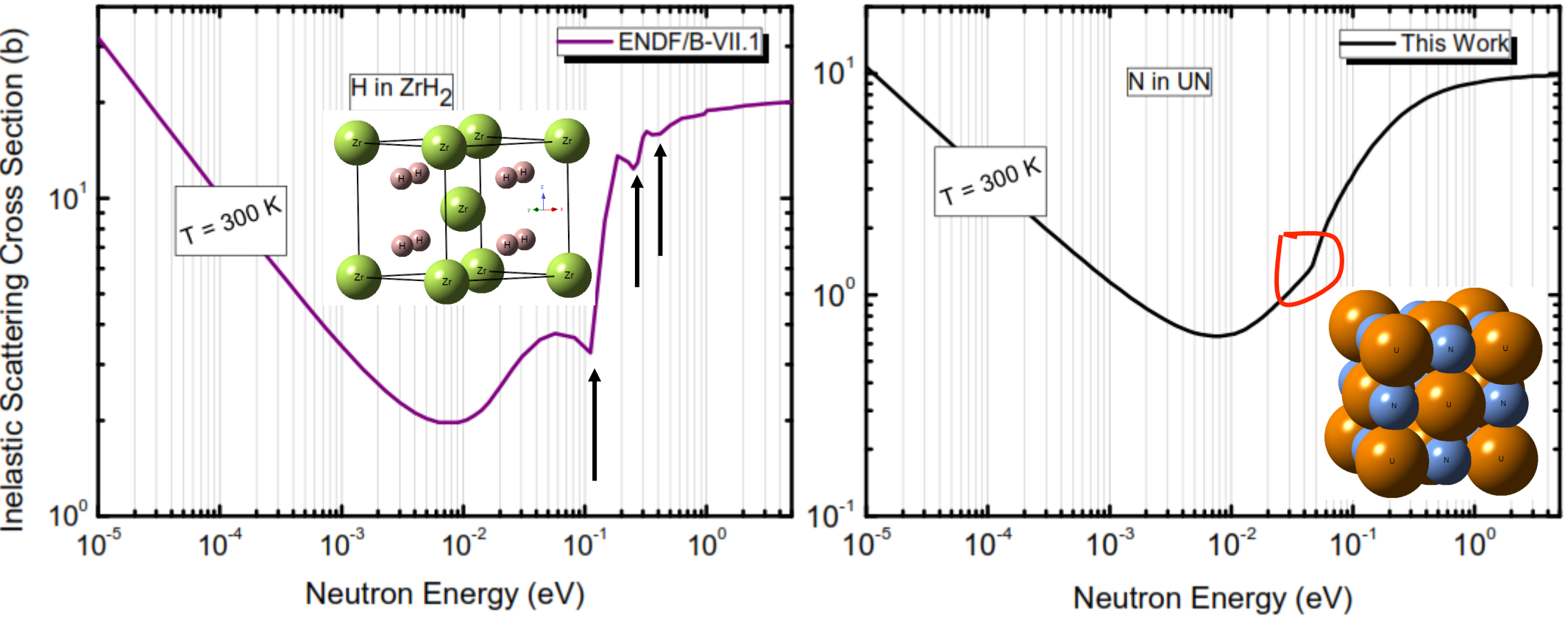
Tetragonal structure H-H interactions ➔ Low potential barrier	Anisotropic Anharmonic
Uneven spacing	

Cubic structure Weak N-N interactions ➔ High potential barrier	Isotropic Harmonic
Even spacing	





N in UN vs H in ZrH_2



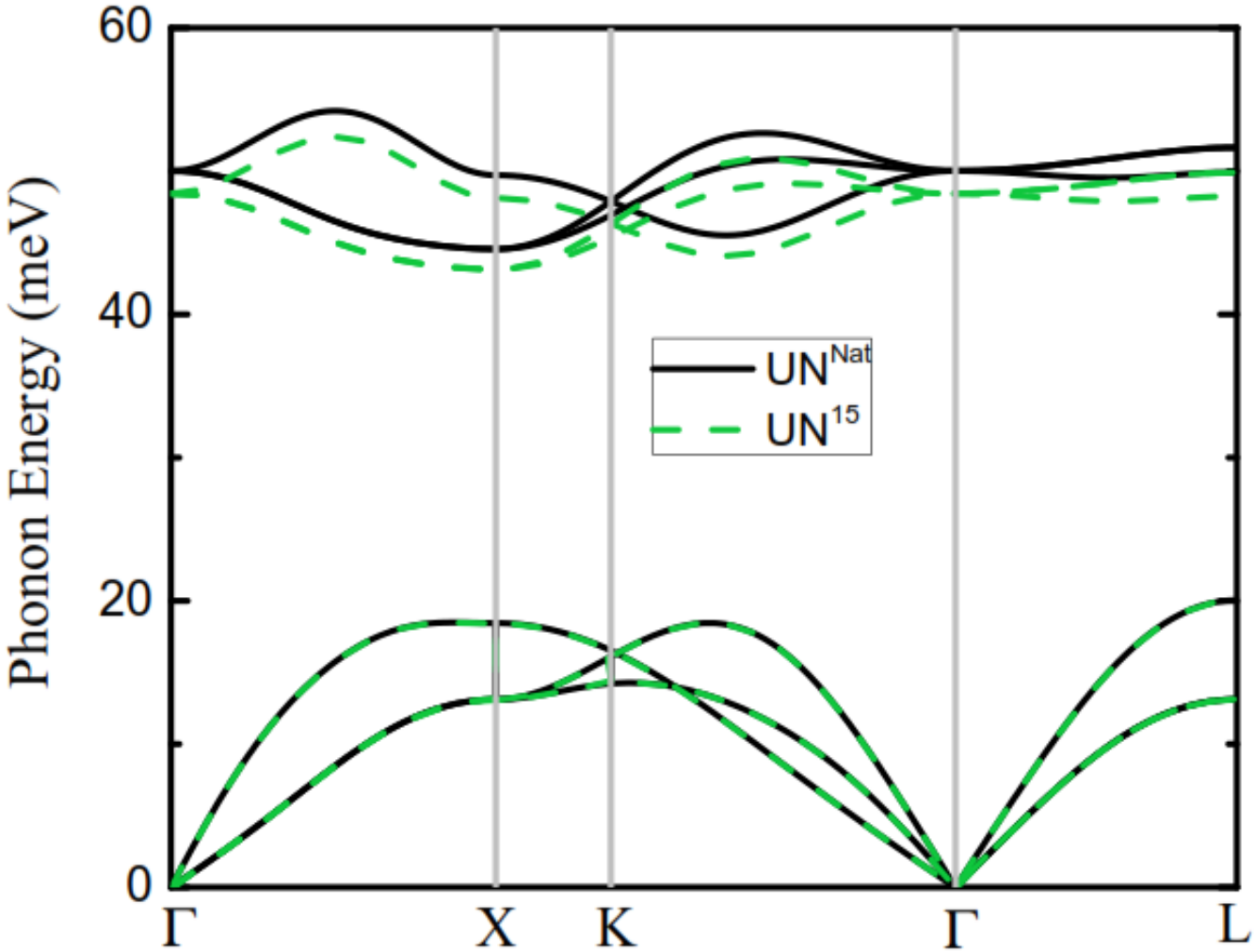
Differential Experiments ➔ constructing and benchmarking libraries

	N^{14}	N^{15}	N^{nat}
%	99.63	0.37	100
A (*u*)	14.003074	**15.000108**	**14.006**

UN^{15}

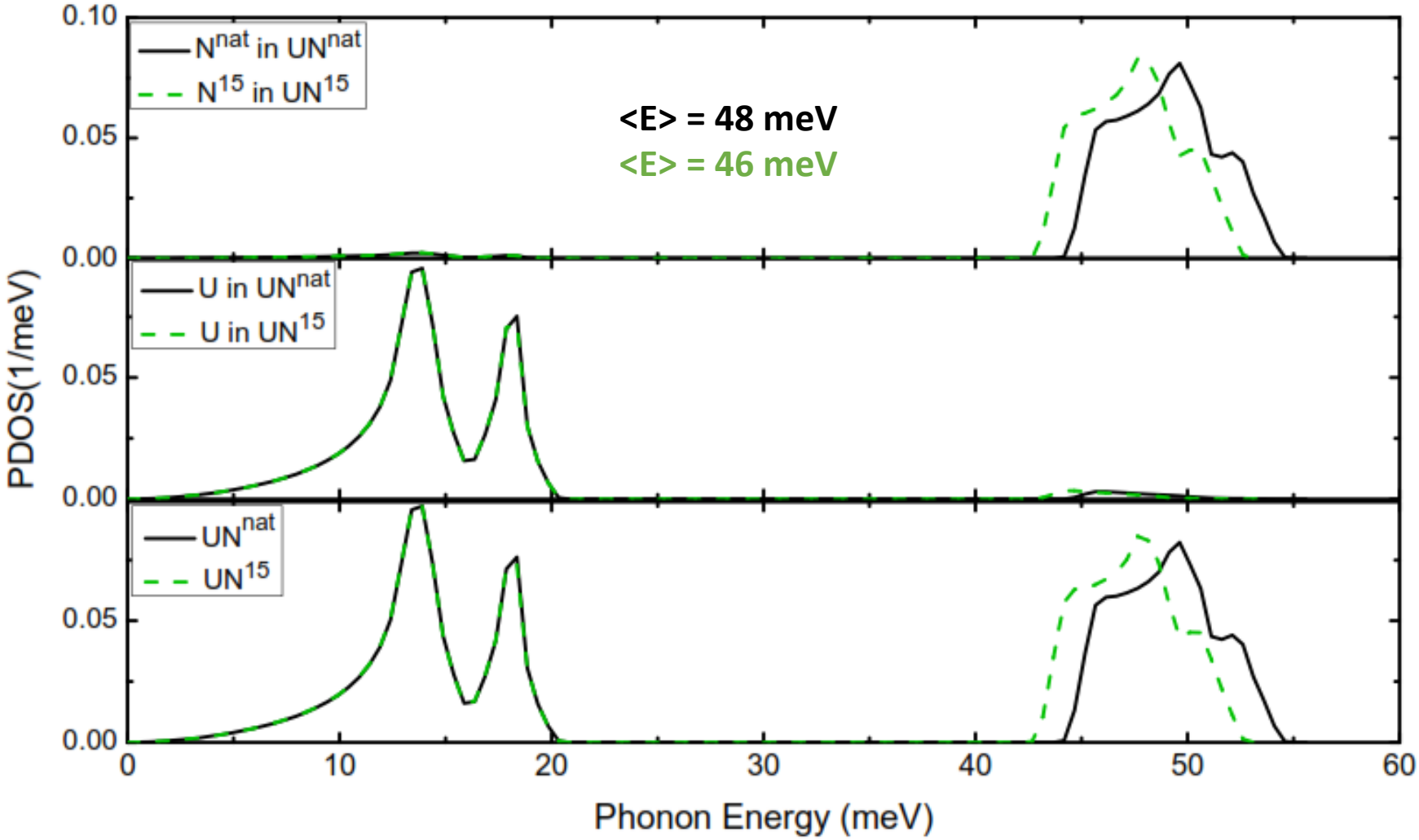
UN^{15} Phonon Dispersion Relations

	N^{14}	N^{15}	N^{nat}
%	99.63	0.37	100
A (*u*)	14.003074	15.000108	**14.006**



UN^{nat} vs UN^{15}

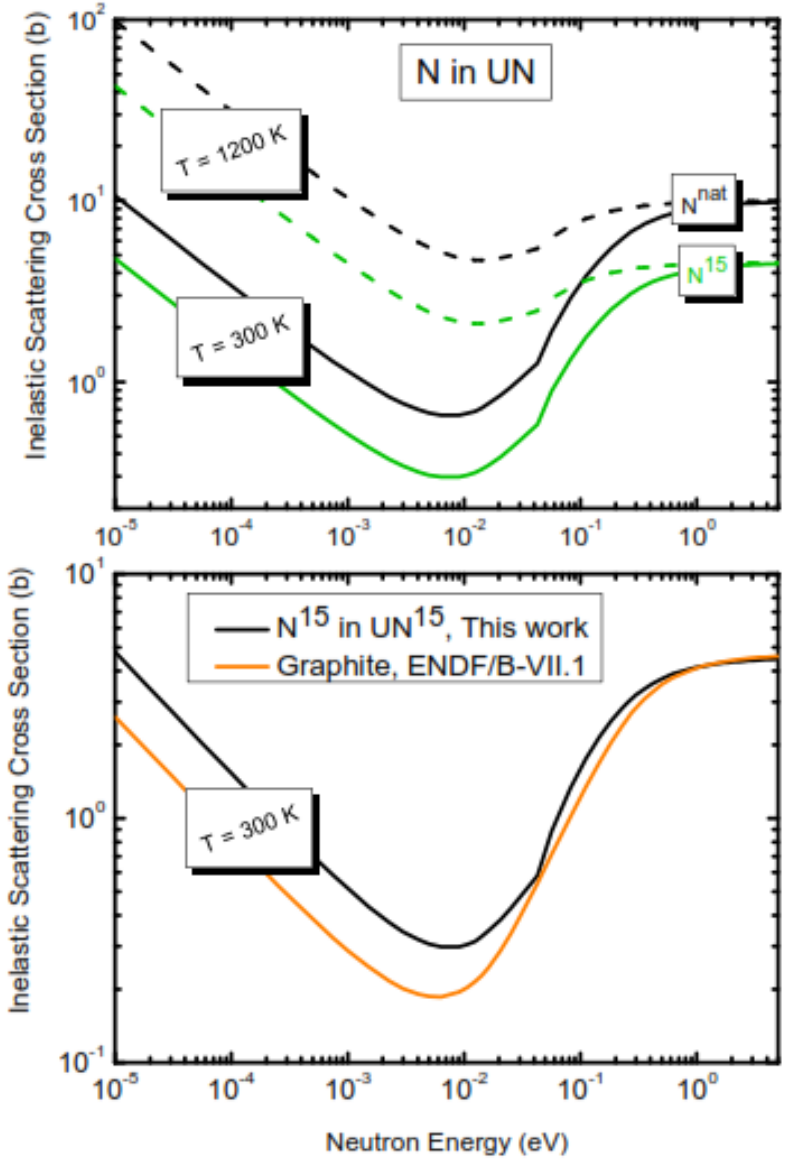
	N^{14}	N^{15}	N^{nat}
%	99.63	0.37	100
A (*u*)	14.003074	15.000108	**14.006**

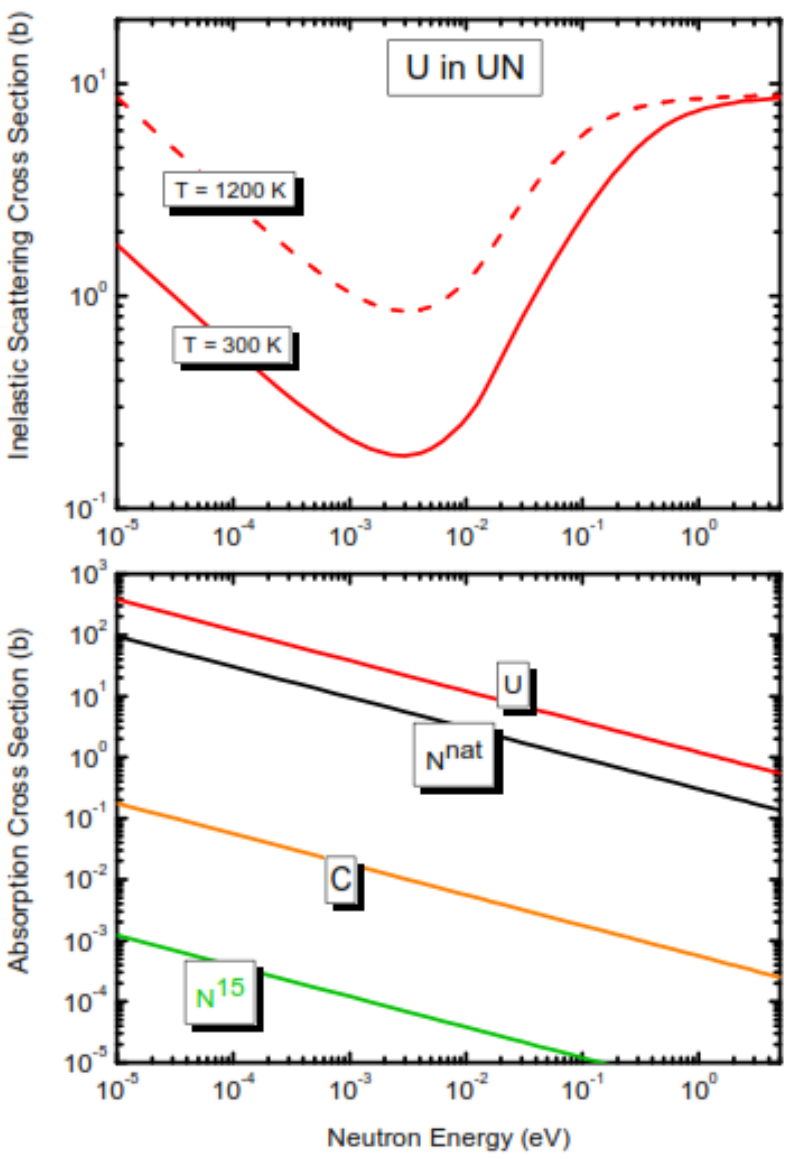


	N^{14}	N^{15}	N^{nat}	U	C	O
s_{coh}	11.03	5.21	11.01	8.903	5.551	4.232
s_{inc}	0.5	0.00005	0.5	0.005	0.001	0.0008
s_b	11.53	5.21	11.51	8.908	5.551	4.232
s_{ab}	1.91	0.000024	1.9	7.57	0.0035	0.00019
%	99.63	0.37				

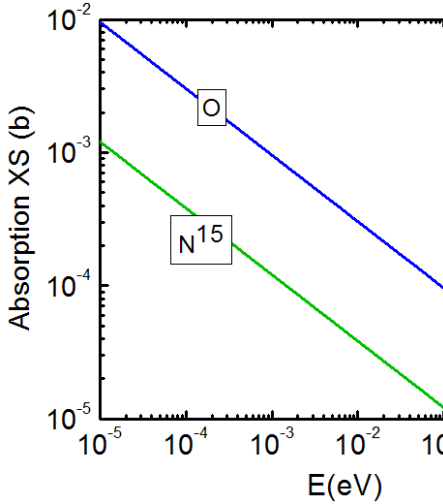
https://www.ncnr.nist.gov/resources/n-lengths/elements/

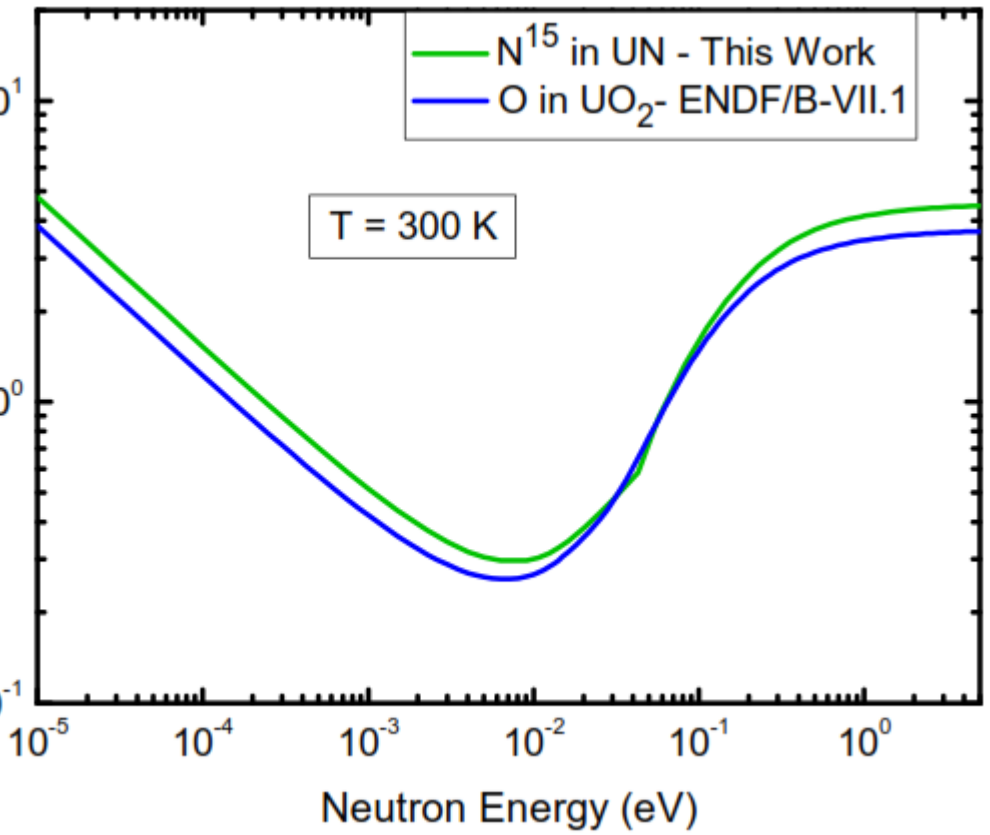
Cross Sections

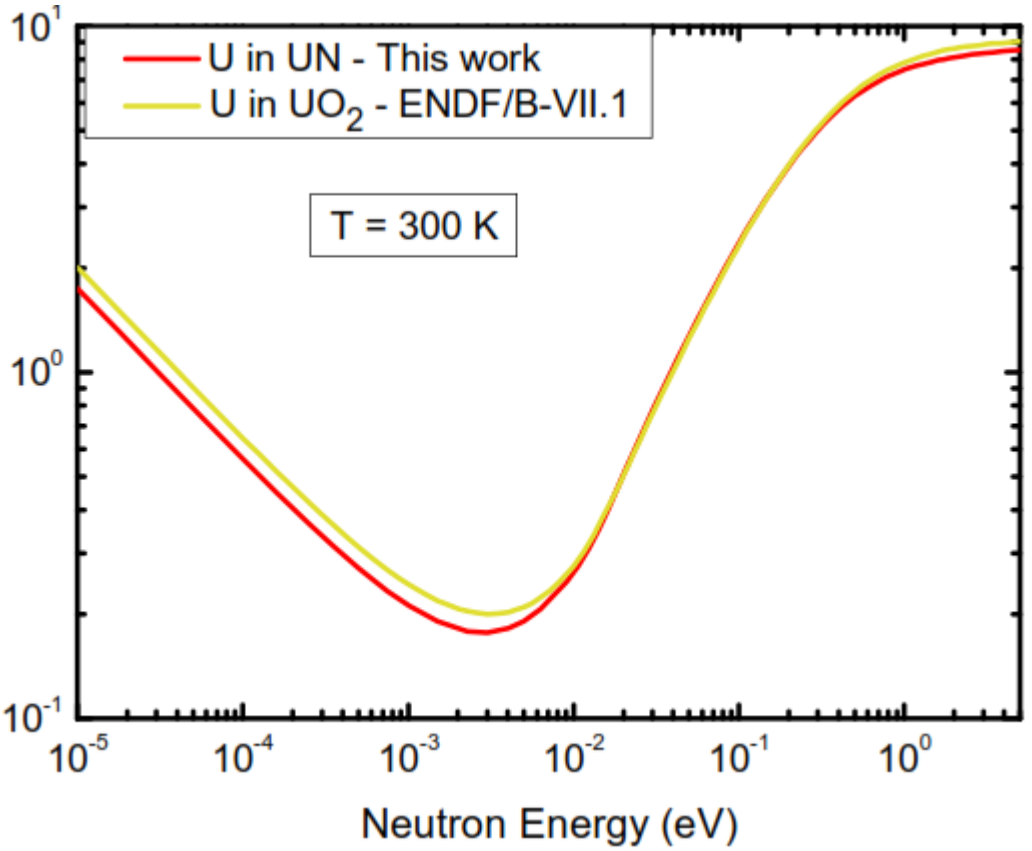




ross Sections:UN^{15} vs UO_2







Conclusion

- An excellent agreement between the calculated and measured phonon dispersion which insures the accuracy of the calculated PDOS

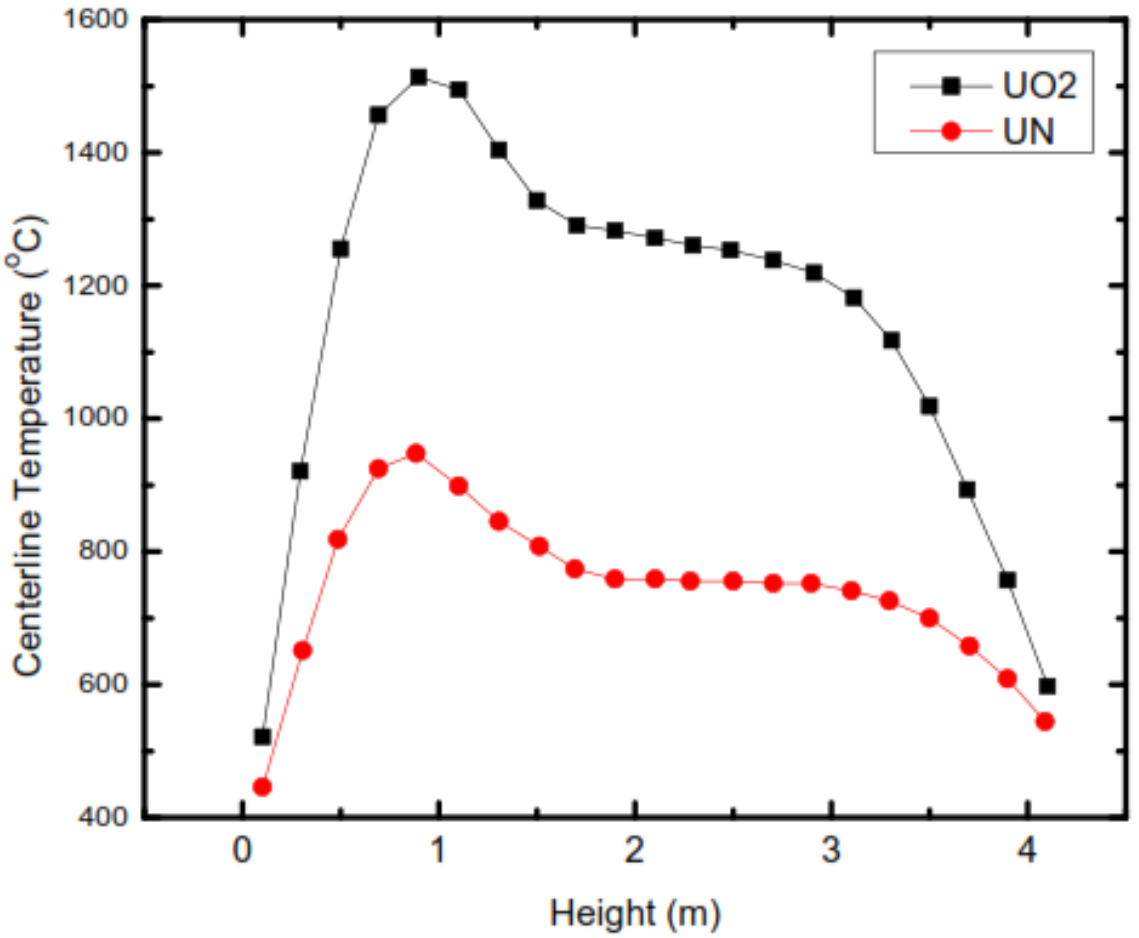
- Unlike H in ZrH_2, the inelastic scattering XS of N in UN does not show variations. For building and benchmarking nuclear data libraries, differential experiments are needed more than integral experiments.

- The inelastic scattering XS of N^{15} is comparable to that of Graphite and O in UO_2

- The UN cross sections calculated in this work represent a future potential ENDF libraries.

Thank You

Motivation



Chaudari et al., 2013. Prog. Nucl. Energy 63, 57-

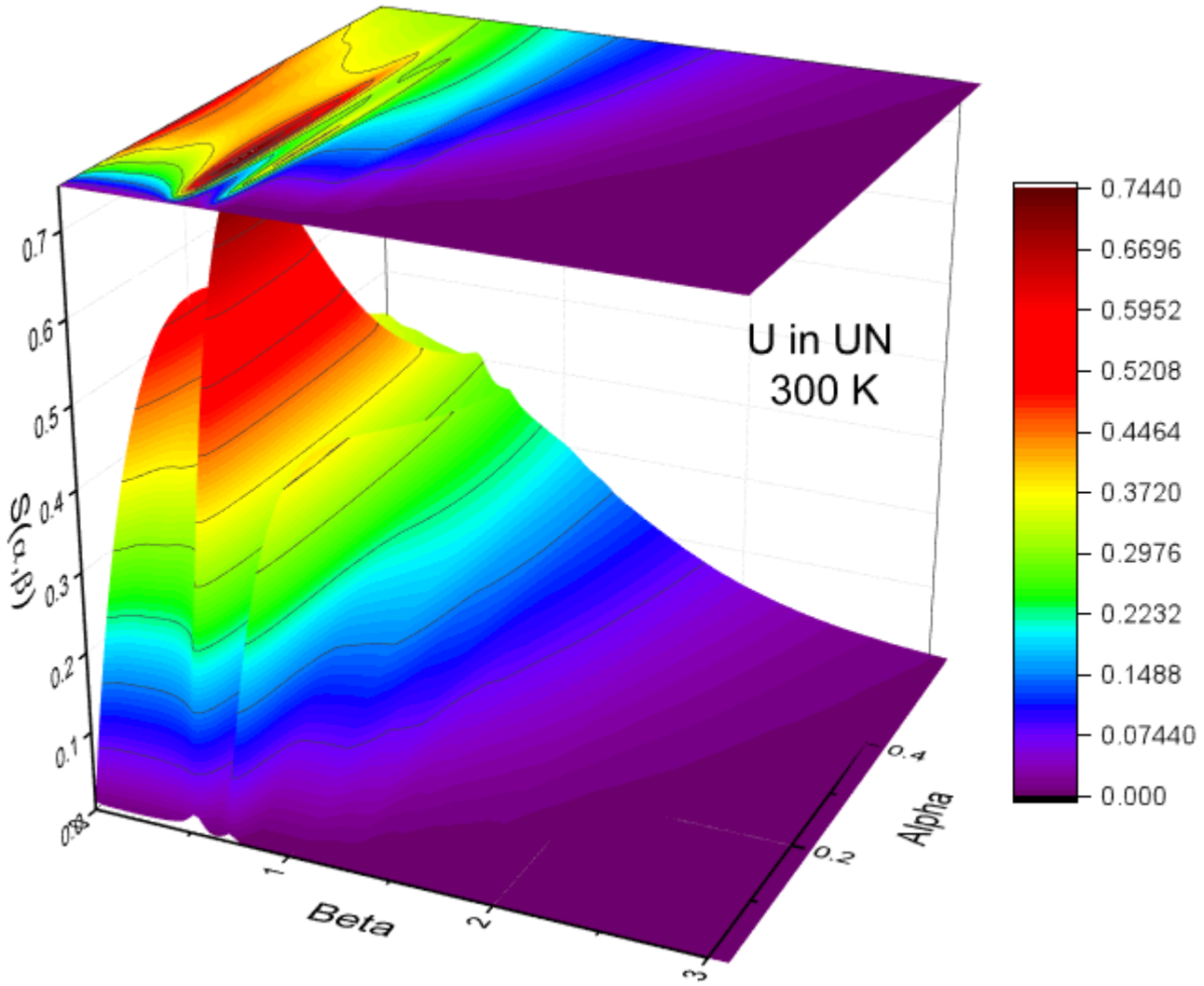
Introduction

- Thermal neutrons have wavelengths comparable to the separation distances of atoms in solids.

➢ As a consequence thermal neutrons are a useful tool in studying the structure of different scattering systems.

- The energy of thermal neutrons is of the same order of magnitude as that of excitations in a scattering medium (e.g., phonons in a solid).

➢ Therefore, thermal neutrons are a useful tool in providing information the dynamics of the scattering medium.


U in UN
300 K
S(q,ω)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.08
Beta
1
2
3
Alpha
0.2
0.4
0.7440
0.6696
0.5952
0.5208
0.4464
0.3720
0.2976
0.2232
0.1488
0.07440
0.000

Mass and Gap effects

$$S(Q,\omega) = \sum_n S_n(Q,\omega)$$

$$S_n(Q,\omega) = \frac{1}{n!}\left(\frac{\hbar Q^2}{2m\omega_o}\right)^n \exp\left(\frac{-\hbar Q^2}{2m\omega_o}\right)\delta(\hbar\omega -$$