The New Thermal Neutron Scattering Measurements and Analysis

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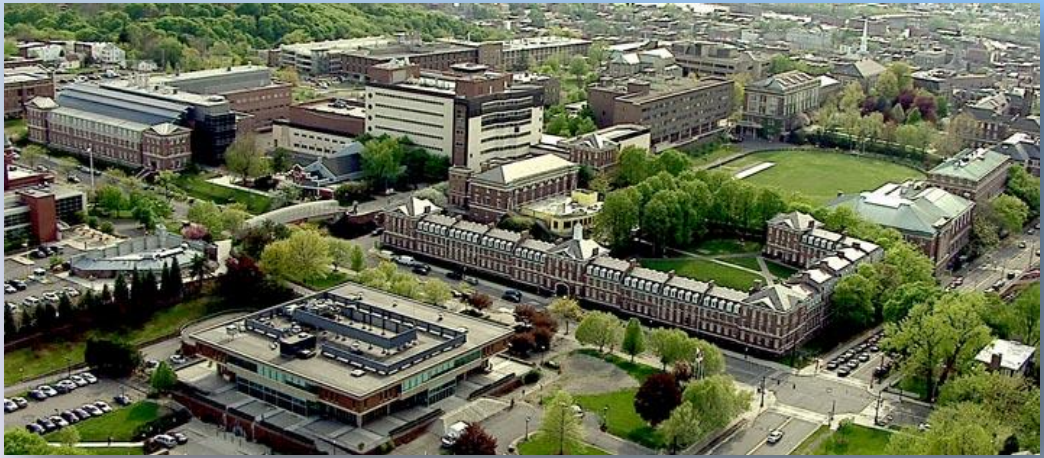

WPEC-SG42 Meeting, Paris, May 15-16, 2018

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Thermal Scattering Experiments Overview

- Overall objectives:
  - **Use double differential thermal scattering and vibrational spectroscopy measurements to benchmark and improve thermal scattering evaluations.**

- Preform measurement at SNS (ORNL):
  - Use ARCS and SEQUOIA for *double differential scattering*.
  - Use VISION for *phonon spectrum measurements*.
    - Key collaborators at ORNL: Goran Arbanas, (Mike Dunn).
    - Scientists at SNS: Alexander Kolesnikov, Doug Abernathy, Luke Daemen, Yongqiang Cheng.

- Advantages:
  - New measurements have much better energy and angle resolution compared to old data.
  - Can measure different type of samples (liquid, solid, mixtures, compounds).
  - Measurements can be done at variety of temperatures starting from 5K.
  - **Tremendous amount of different experimental information helps constrain and overcome modeling deficiencies.**

Completed Experiments

Moderators	SEQUOIA (Ω: 3-58º in 1º increments)	ARCS (Ω: 3-125º in 1º increments)	VISION (at 5 K)
Light Water (H_2O)	E_I: 55, 160, 250, 600, 1000, 3000, 5000 meV Temp: 300 K		YES
Polyethylene (CH_2)	E_I: 55, 160, 250, 600, 1000, 3000, 5000 meV Temp: 300 K	E_I: 50, 100, 250, 700 meV Temp: 5, 295 K	YES
Quartz (SiO2)		E_I: 50, 100, 250, 700 meV Temp: 5, 295, 573, 823, 873 K Thickness: 3.175, 6.35 mm	YES
Teflon ($(C_2F_4)_n$)		E_I: 50, 100, 250, 700 meV Temp: 5, 300, 500 K	NO
Lucite ($C_5O_2H_8$)		Ei: 50, 100, 250, 700 meV Temp: 5, 300, 400 K	YES
Concrete (mixture)		Ei: 50, 100, 250, 700 meV Temp: 5, 300 K	NO

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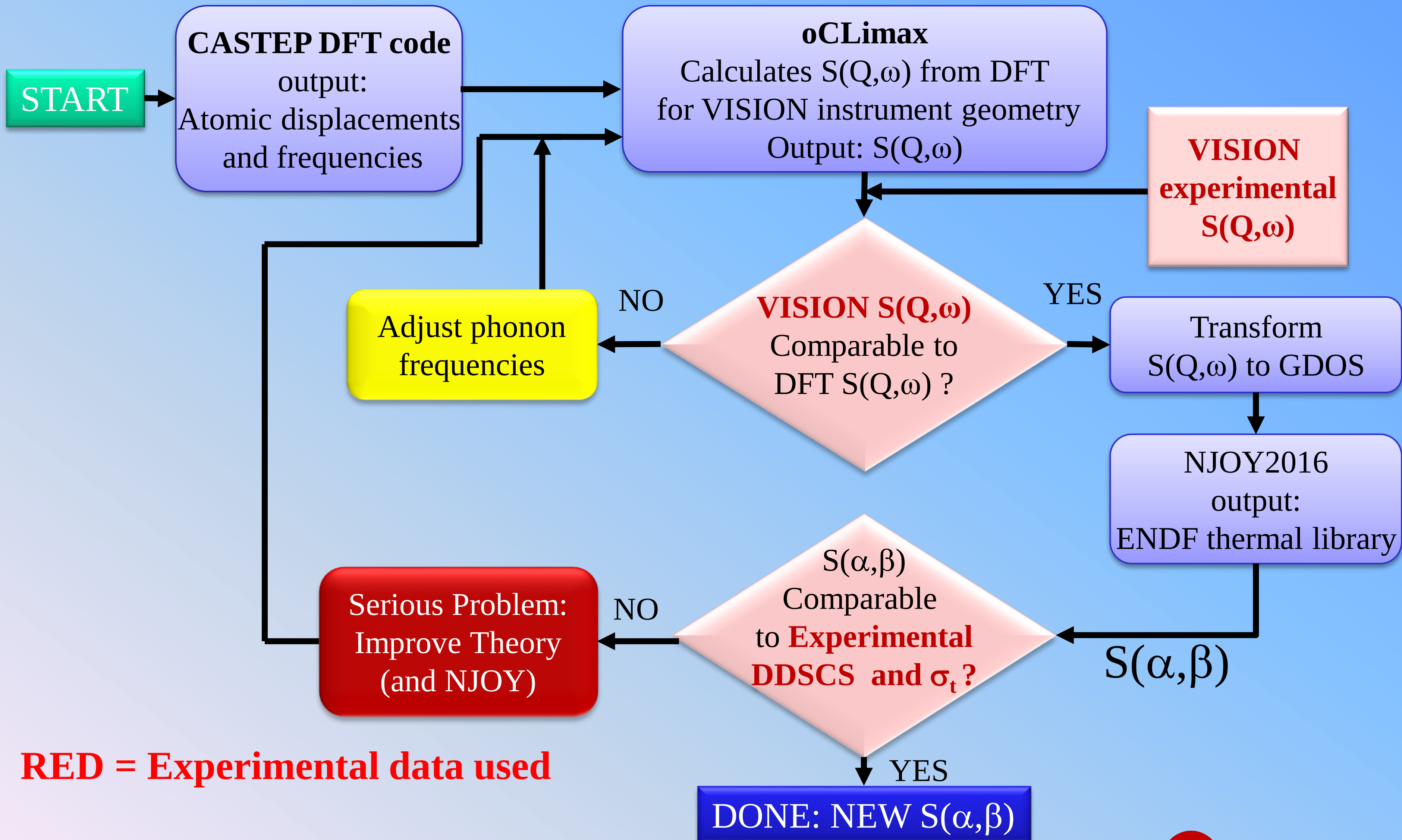
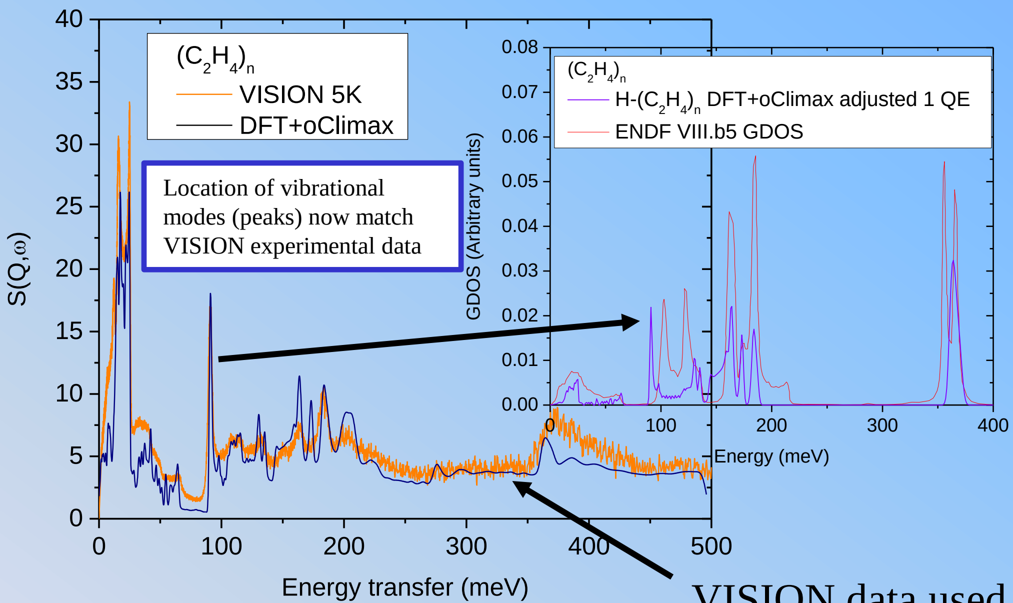
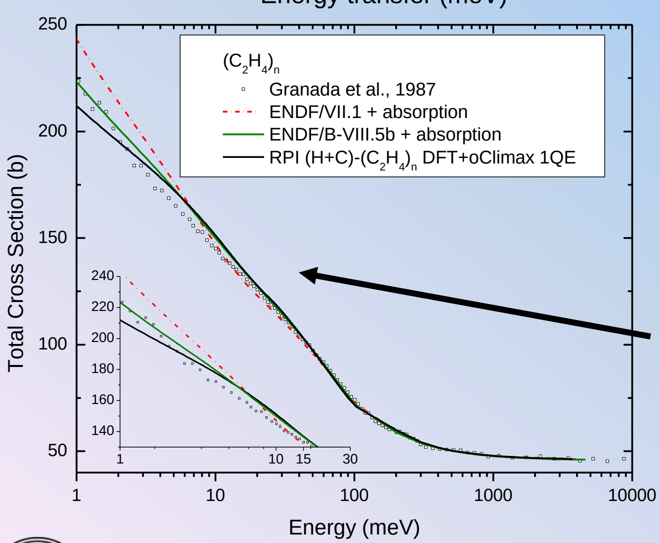
Thermal scattering – evaluation methodology



RED = Experimental data used

Polyethylene Experimental Data and Evaluation

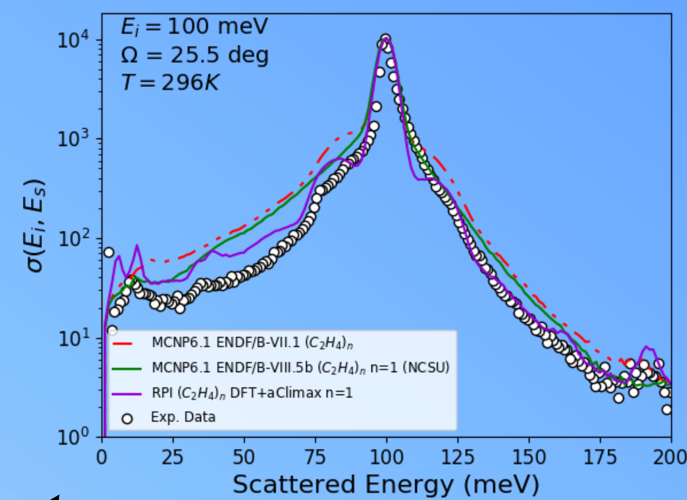


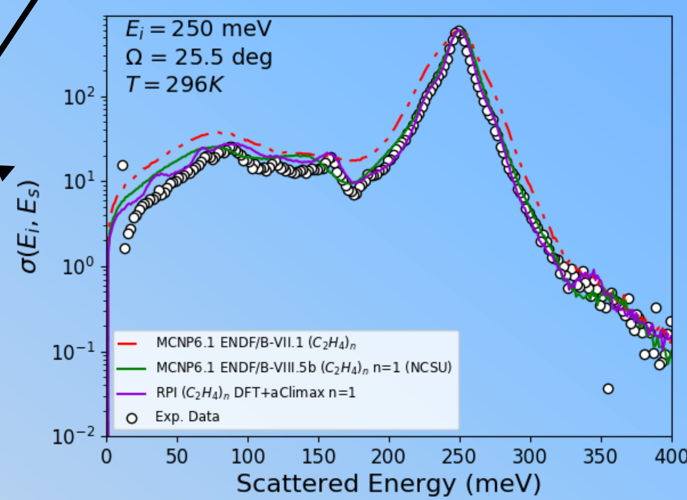


VISION data used to validate and adjust the evaluation

Experimental data used for validation:

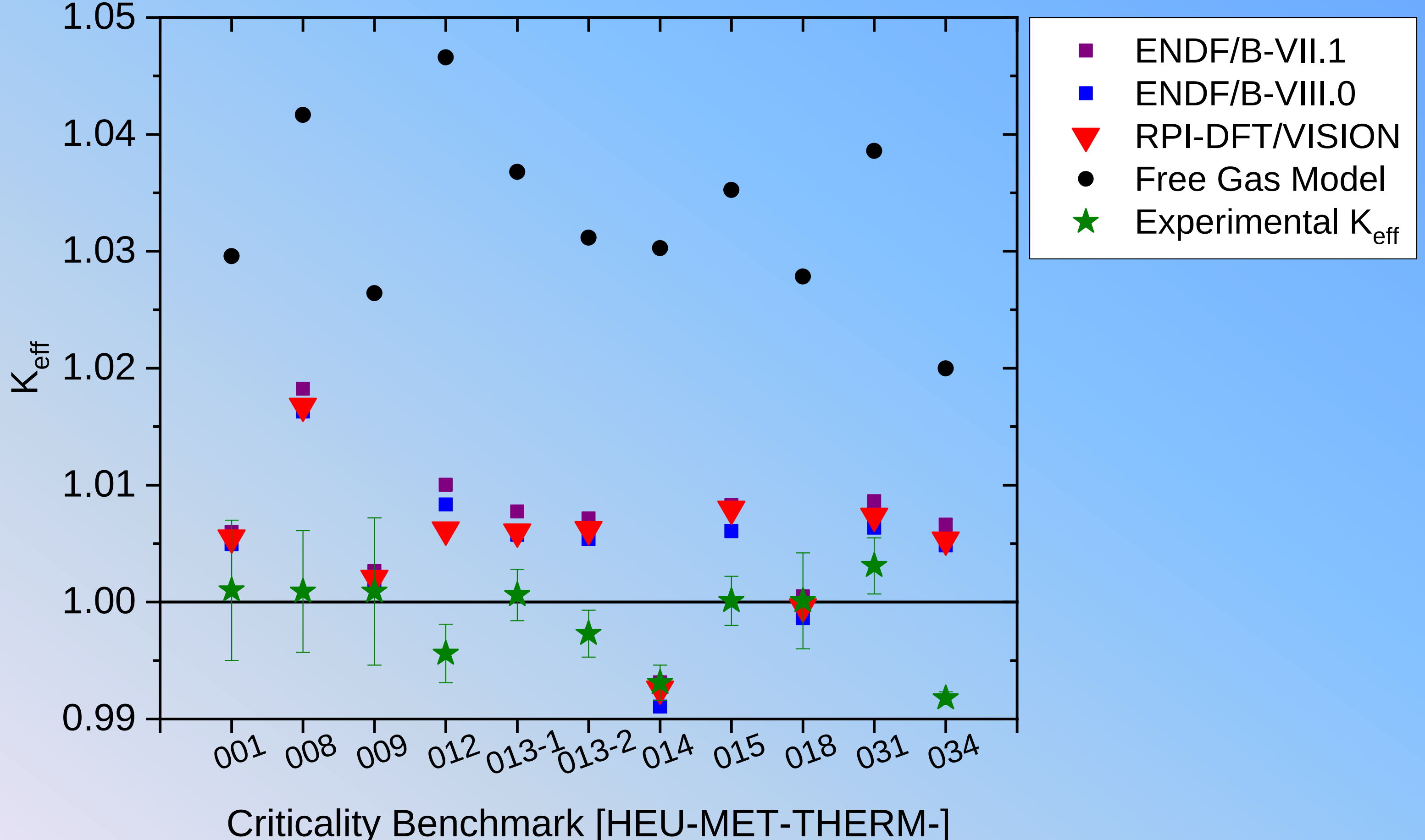
- Double differential scattering
- Total cross section from the literature





Polyethylene Criticality Benchmarks

- The new RPI evaluation and the ENDF/B-VIII.0 give similar results.
- There are some discrepancies between the benchmarks and simulation.



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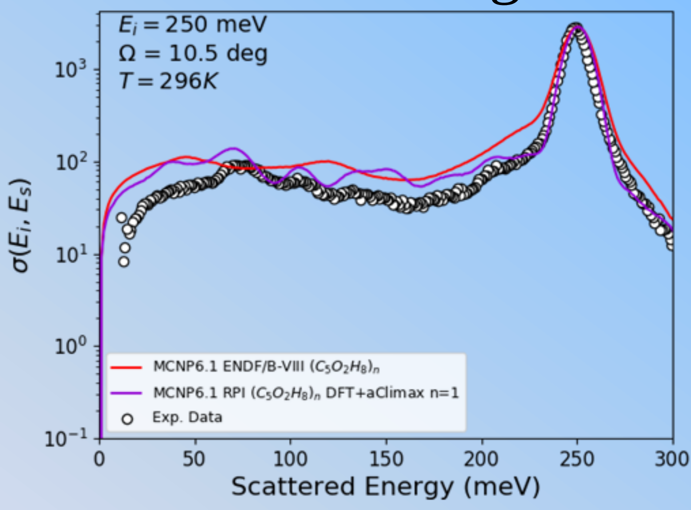
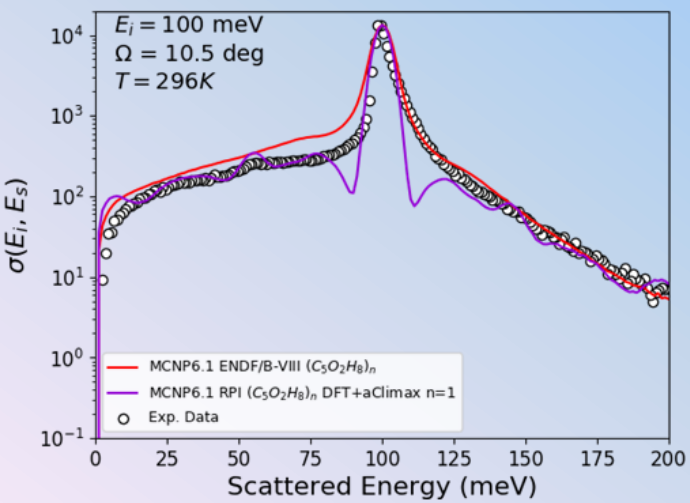
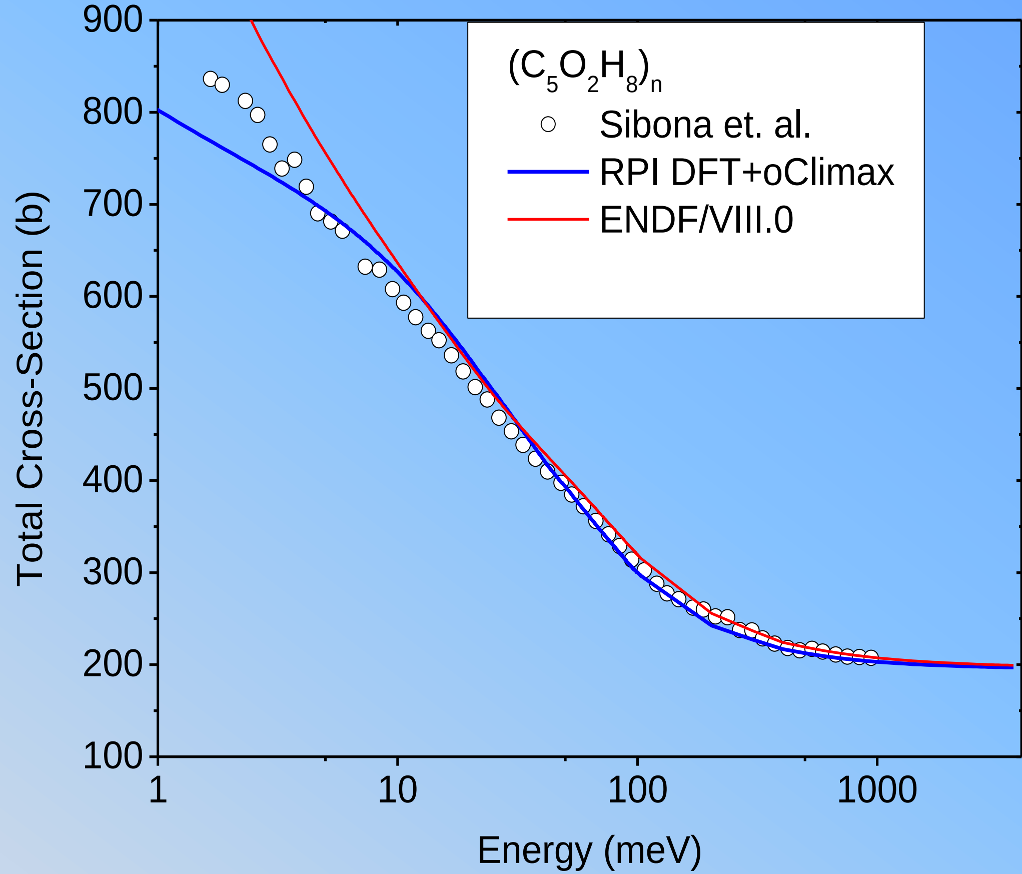
Lucite ($C_5O_2H_8$) DDSCS

- ENDF/B-VIII.0 gives better representation of inelastic region

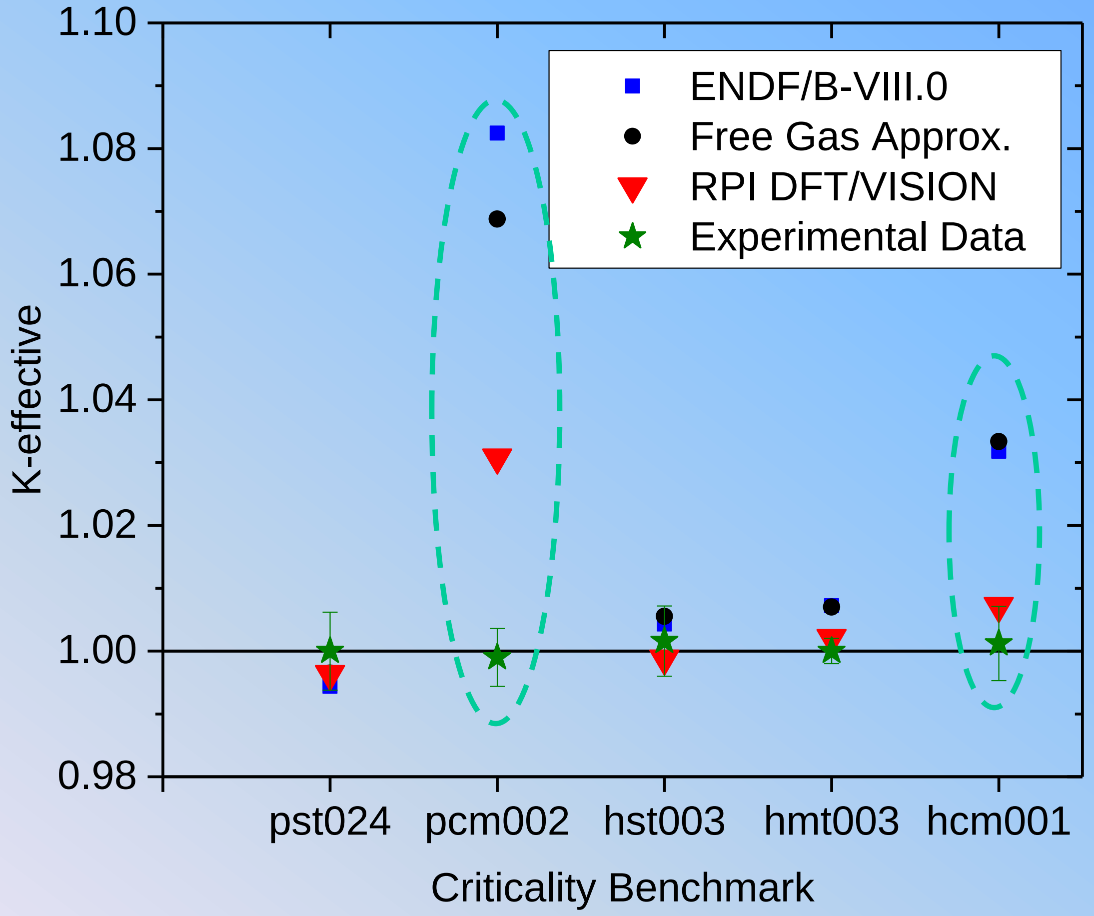






Lucite Criticality Benchmarks

- RPI TSL file represents a clear improvement to K-effective
- ENDF/B-VIII.0 is similar to free gas treatment



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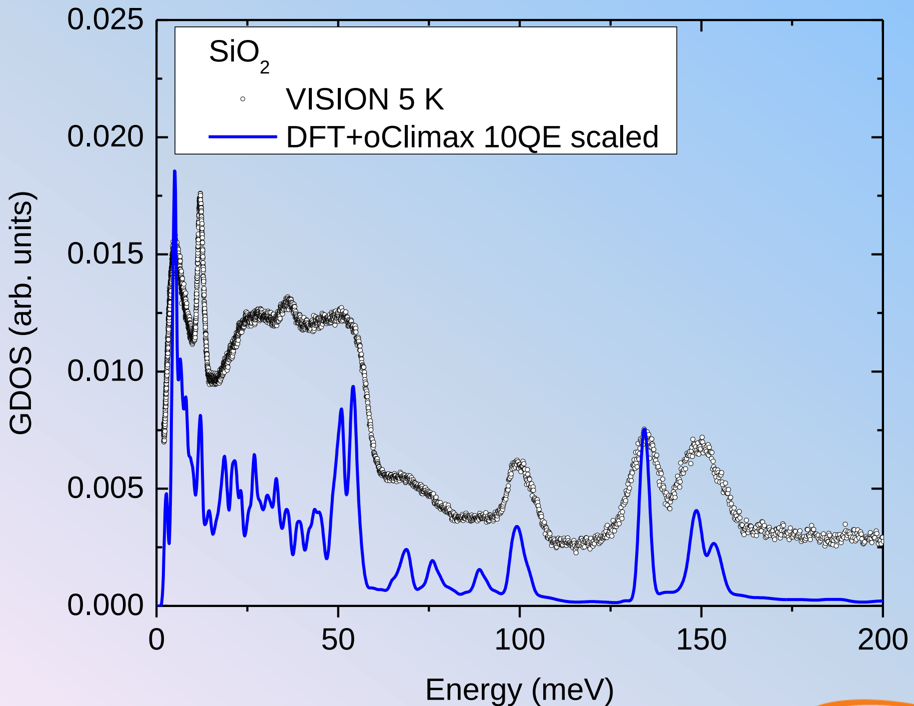
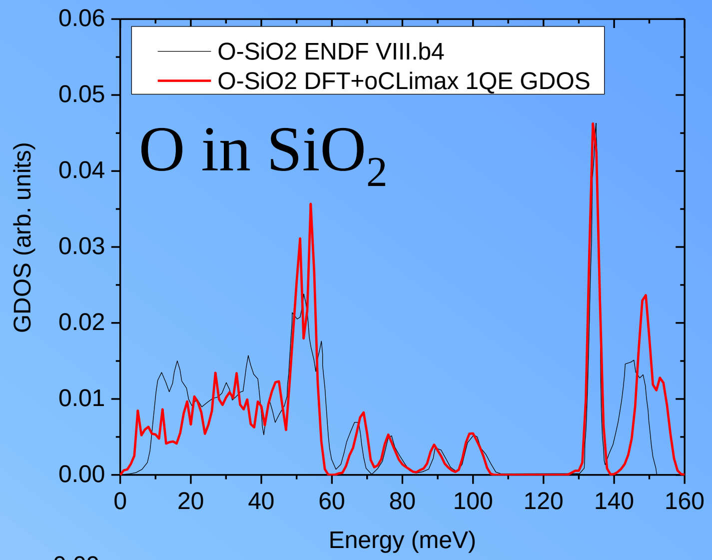
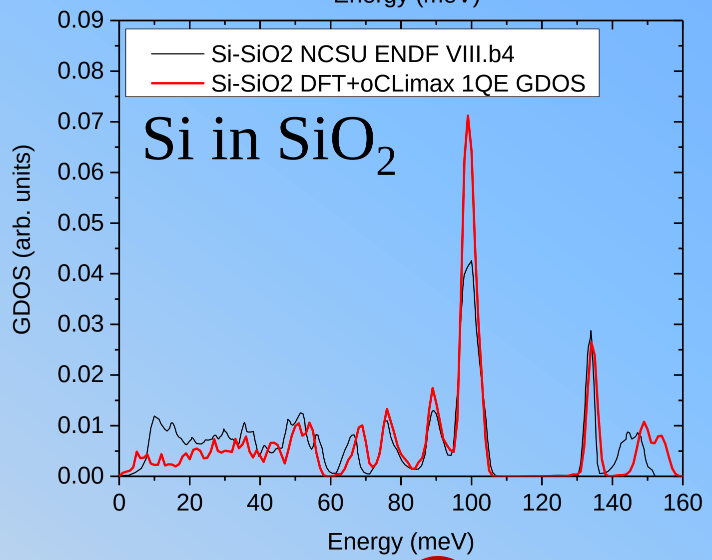
Quartz Evaluation

- Use VISION data to fine tune mode locations.
- Separate files for Si and O







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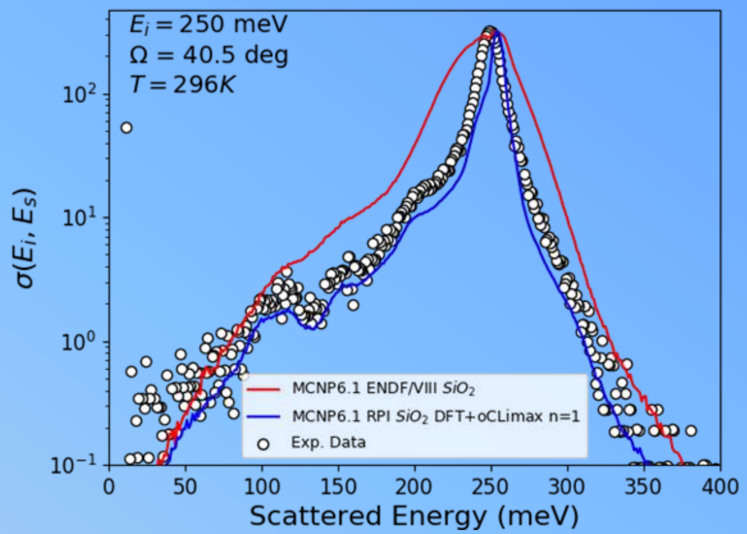
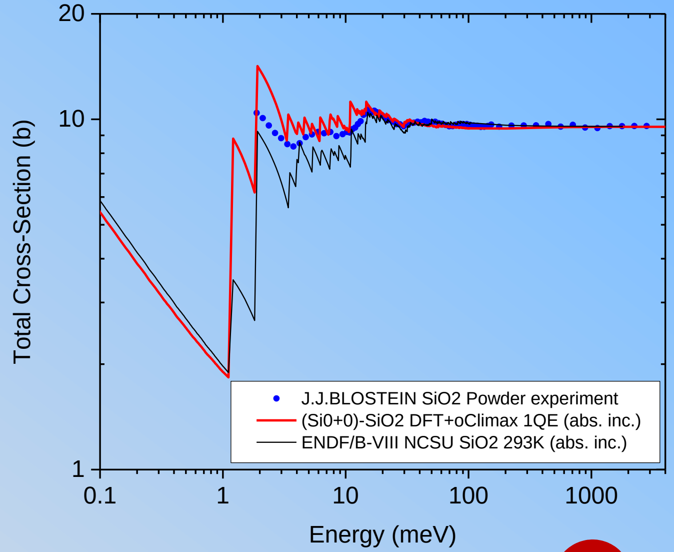
Quartz Evaluation

- The RPI evaluation is in better agreement with the differential scattering experiment



- Arguably better agreement with the literature total cross section below 15 meV



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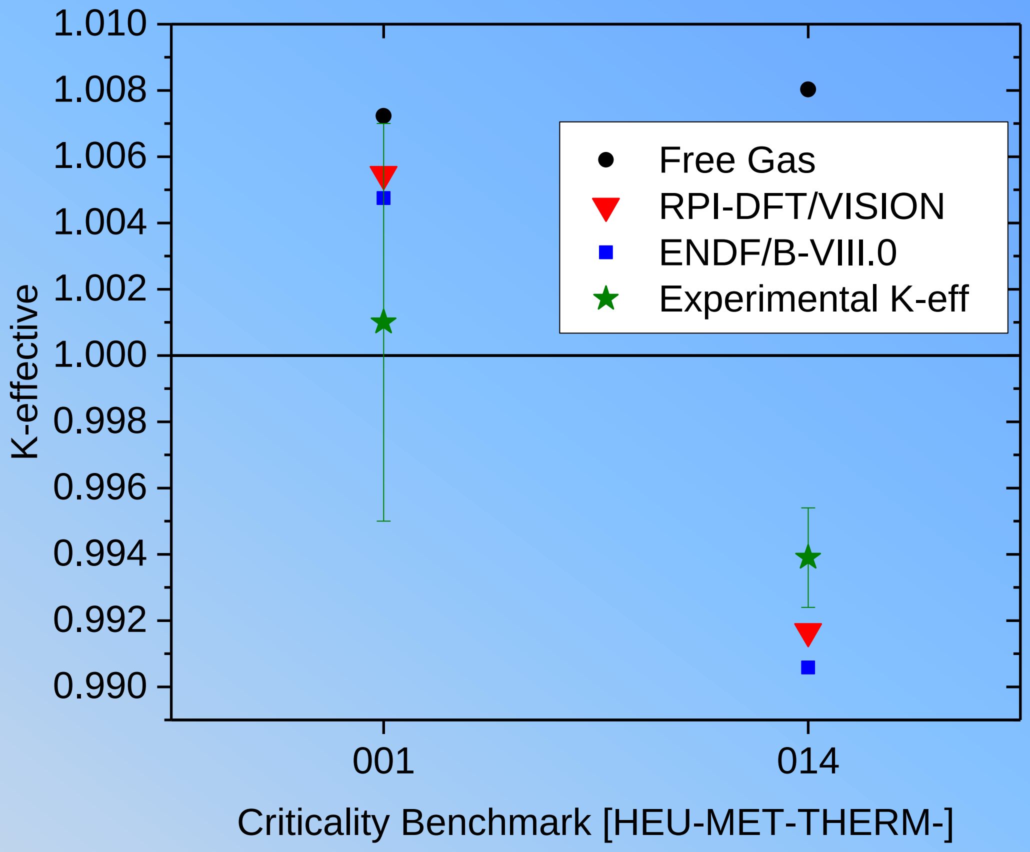
Quartz Criticality Benchmarks

- Found only two sensitive benchmarks
- ENDF/B-VIII.0 and the RPI evaluation show similar performance for HEU-MET-THERM-001 which is close to free gas (low sensitivity to S(α,β))
- The RPI evaluation is slightly better when there is high sensitivity to thermal scattering (HEU-MET-THERM-014)



Progress of Concrete

Experiment vs. Library (pick which one?)

- DDSCS (Double Differential Scattering Cross Section)
- Benchmark K_{eff}

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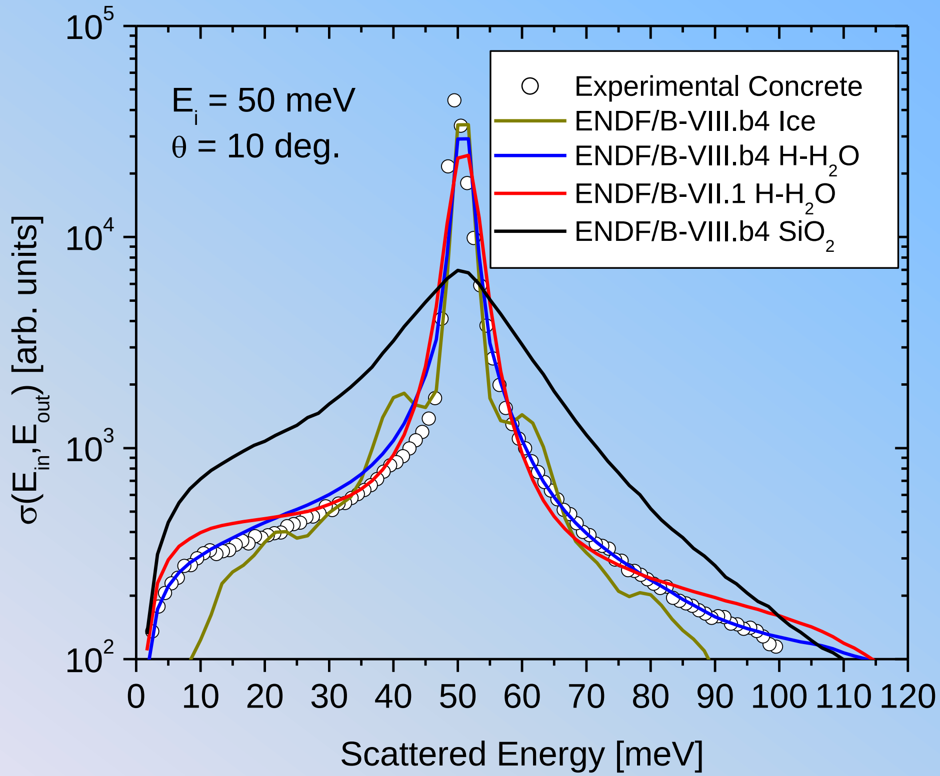
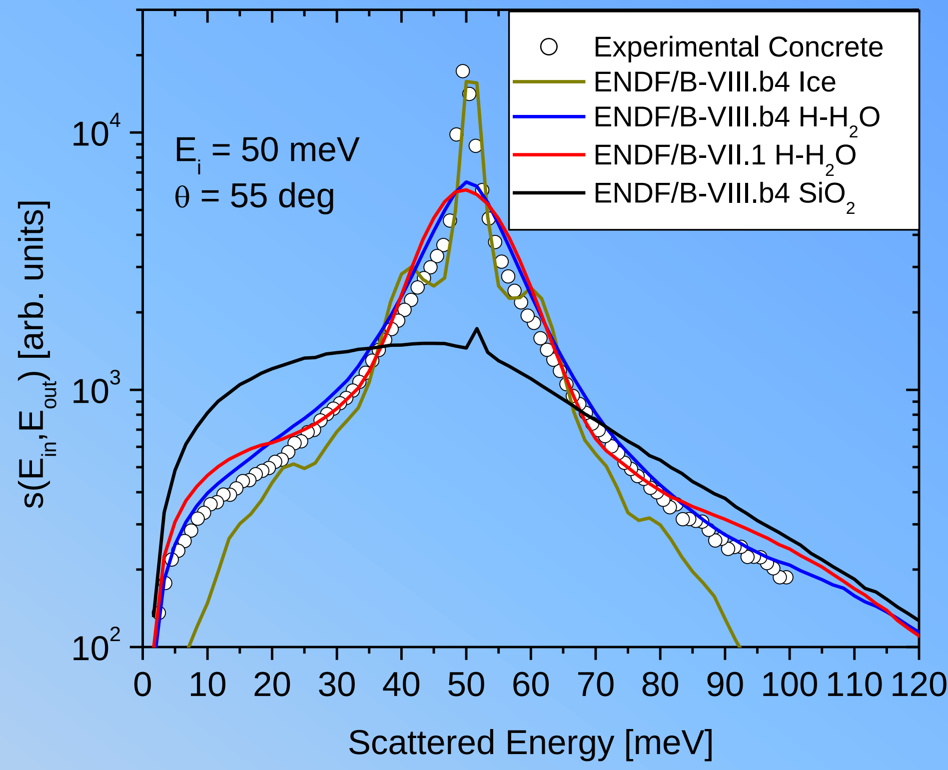
Concrete DDSCS – Single TSL File





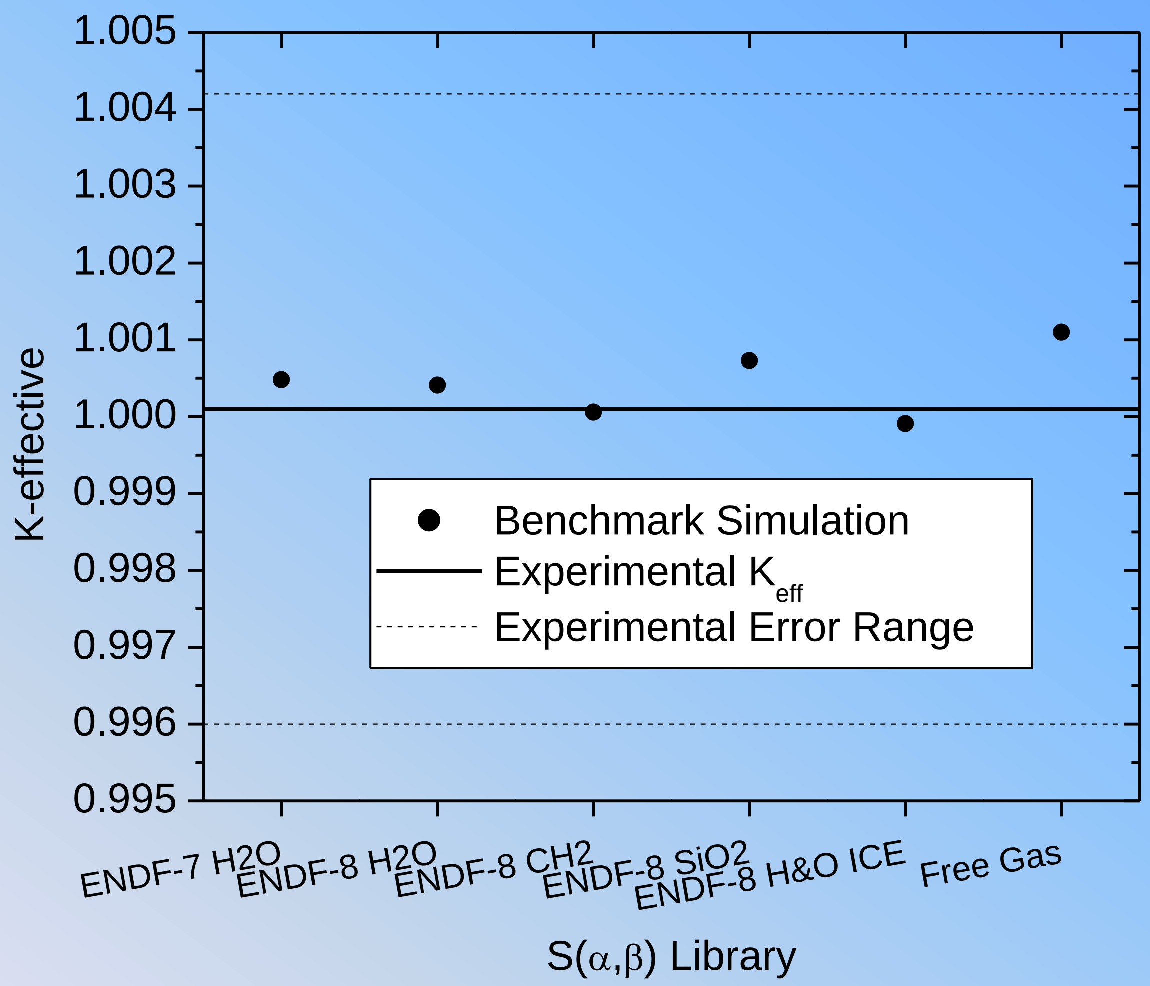
- At 10 deg., ice and liquid water show good representation of shape
- Water's representation of the elastic peak decreases as angle increases, while ice is consistent

Concrete Criticality Benchmark

- International Handbook of Evaluated Criticality Safety Benchmark Experiments (Dice)
  - HEU-MET-THERM-018
  - SiO_2 & Free Gas are the simulations off from about 1 standard deviation

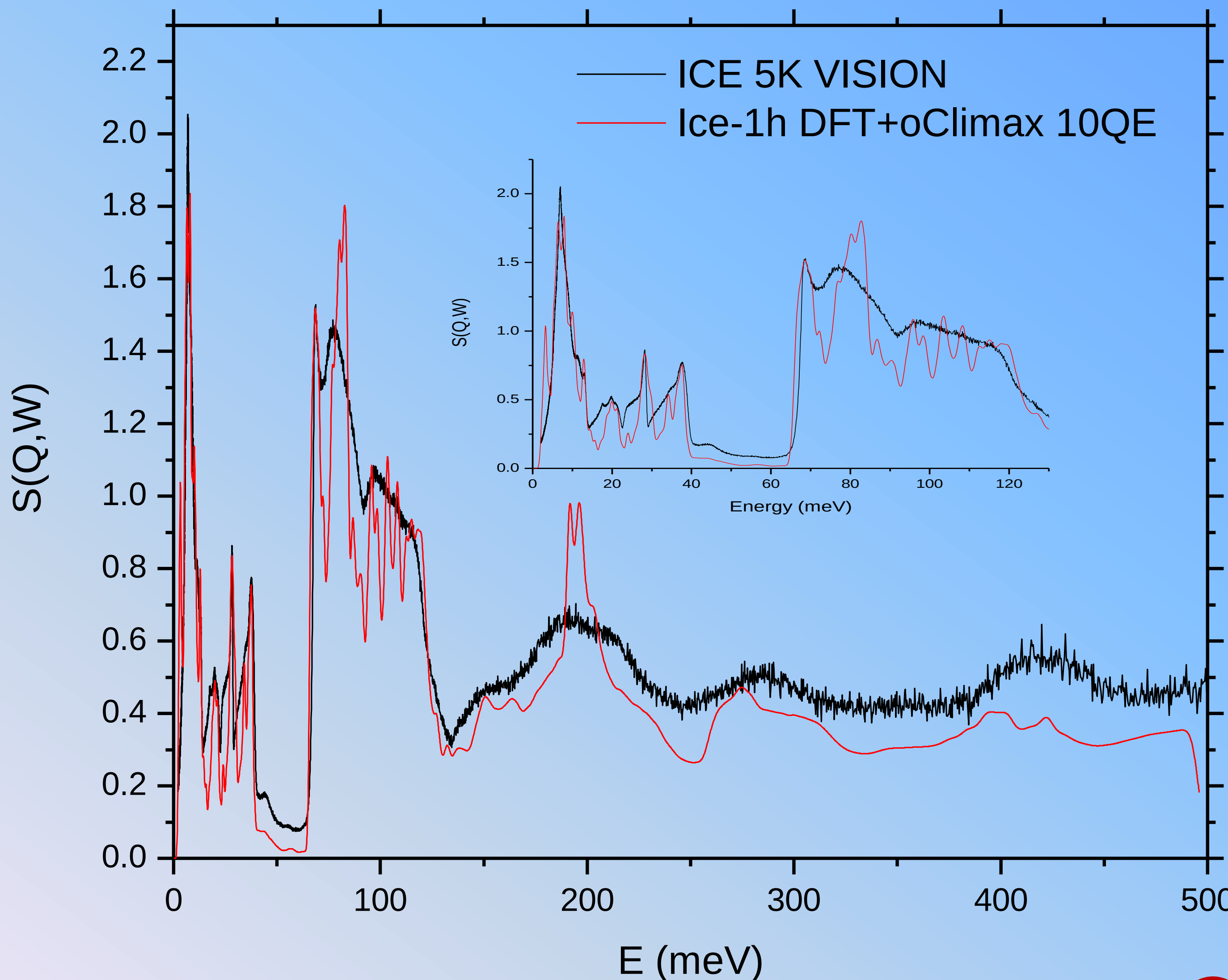
S(α,β) (all other libraries are ENDF/B-VII.1)	**K_{eff}**	**Standard Deviation**
ENDF/B-VII.1 H_2O	1.00048	0.00035
ENDF/B-VIII.b4 H_2O	1.00041	0.00037
ENDF/B-VIII.b4 CH_2	1.00006	0.00035
ENDF/B-VIII.b2 SiO_2	1.00073	0.00036
ENDF/B-VIII.b4 H-ICE	0.99998	0.00035
ENDF/B-VIII.b4 H&O-ICE	0.99991	0.00035
Free Gas (No S(α,β))	1.00110	0.00035
Experimental	1.0001	0.0041

Concrete Criticality Benchmark



- Bound hydrogen models (CH_2 and Ice) give the best representation

Ice Phonon Spectrum



2018 related publications

Journal

1. Kemal Ramić, Carl Wendorff, Yongqiang Cheng, Alexander I. Kolesnikov, Doug L. Abernathy, Luke Daemen, Goran Arbanas, Luiz Leal, Yaron Danon, and Li (Emily) Liu, "Thermal Scattering Law of $(C_2H_4)_n$: Integrating Experimental Data with DFT Calculations", reply to reviews submitted, Annals of Nuclear Energy, 2018.
2. Carl Wendorff, Kemal Ramic, Alexander I. Kolesnikov, Douglas L. Abernathy, Yaron Danon, Li (Emily) Liu, "Improved experimental data and analysis for accurate thermal scattering kernel evaluations of neutron moderators", in final review.

Thesis

1. Kemal Ramić, "From Experiments to DFT Simulations: Comprehensive Overview of Thermal Scattering for Neutron Moderator Materials", Defended and thesis to publish in August, 2018.
2. Carl Wendorff, "Validation and Benchmarking of the Thermal Neutron Scattering Law Data Files for Neutron Moderators using Experimental Data", to defend in June and thesis to publish in August, 2018.

Acknowledgement

- Key collaborators: Goran Arbanas, Luiz Leal, Mike Dunn.

- Special thanks to the help from scientists at SNS:

Alexander Kolesnikov, Doug Abernathy, Luke Daemen, Yongqiang Cheng

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Thanks! Questions?

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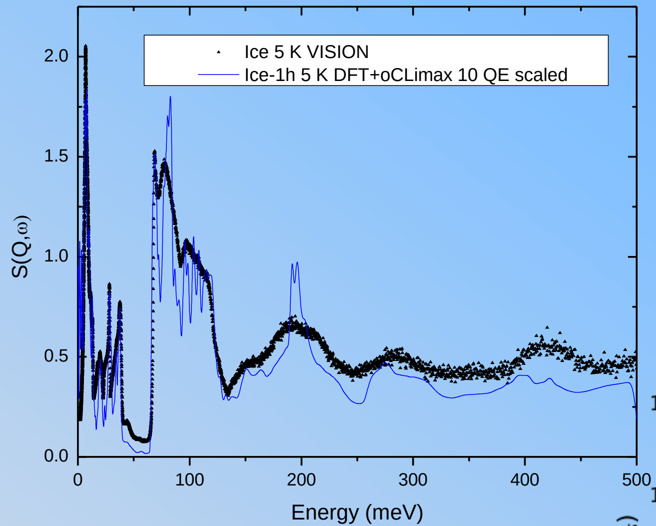
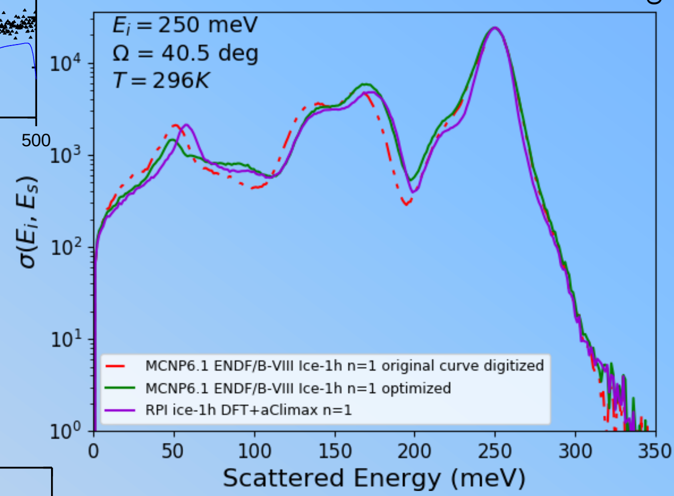
Additional Slides

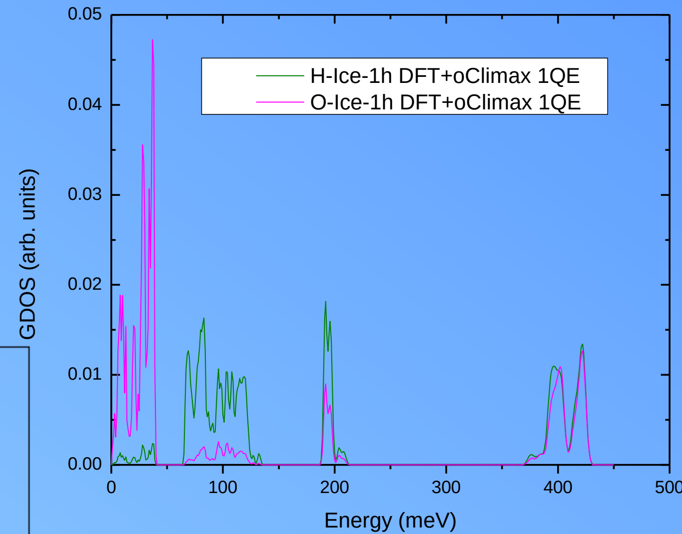
Observation

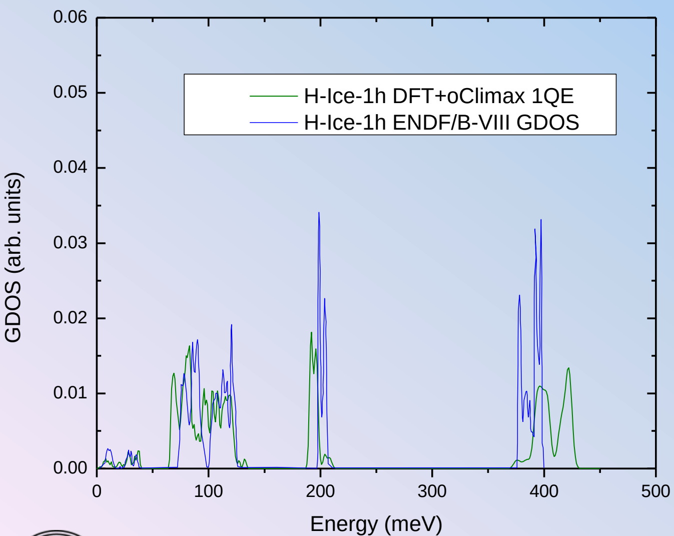
Most of the times we assume the materials have perfect crystalline structure, but with new methodology (including measurements from VISION) we can determine how much measured material deviates from the perfect structure.

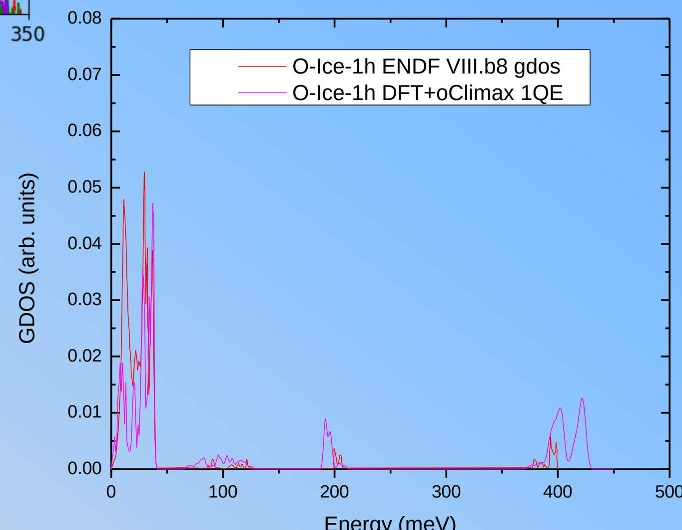
Ice-1h (H_2O)
VISION method











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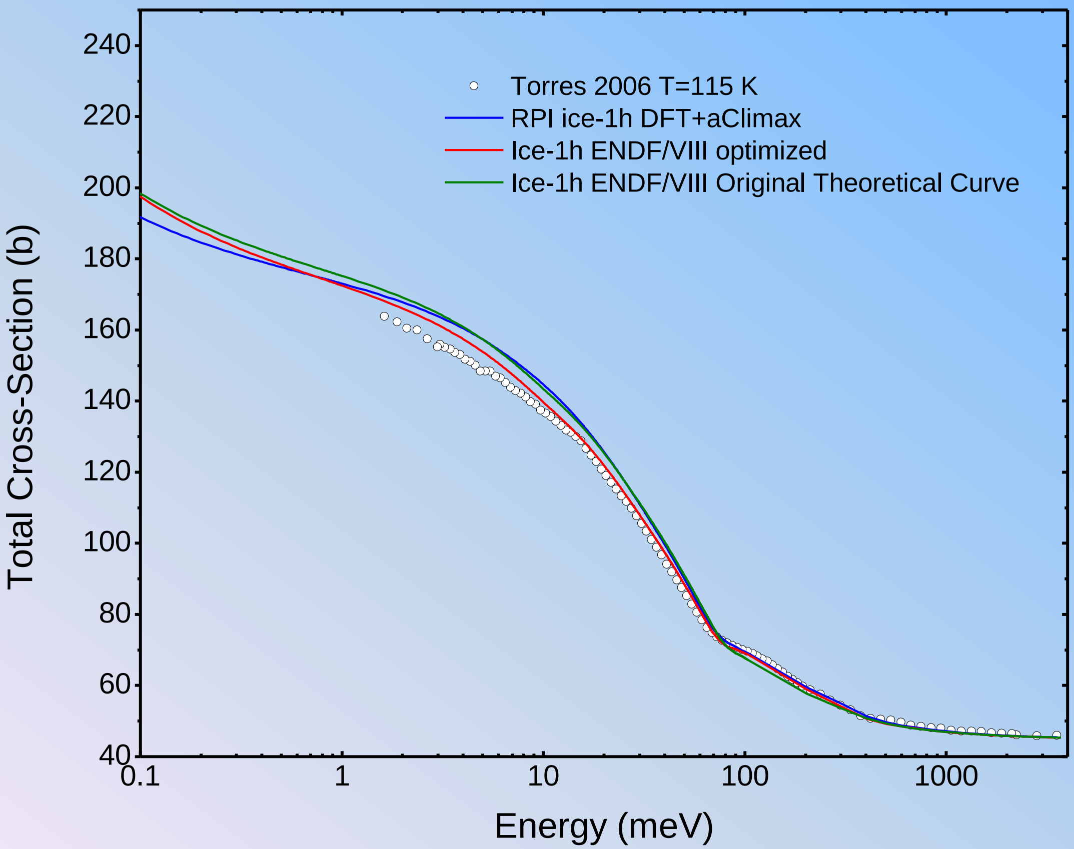
Ice-1h (H_2O)
Total cross section

$$\sigma(H_2O,t] = 2\times(\sigma_{H,s}^{NJOY\ 2016} + \sigma_{H,\gamma}^{NJOY\ 2016}) + (\sigma_{O,s}^{NJOY\ 2016} + \sigma_{O,\gamma}^{NJOY\ 2016})$$



- The RPI library performs better in the region below 1 meV and above 70 meV.
- The RPI library would benefit from the same optimization as ENDF library.

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