Towards a better thermal neutron scattering law generation: oClimax + NJOY2016

K. Ramic, C. Wendorff, J. Hou, J. Feng, Y. Danon, E. Liu

Rensselaer Polytechnic Institute, Troy, NY, 12180

ANS Winter Meeting 2018, Orlando FL, November 2018

Rensselaer

NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

linac The Gaerttner LINAC Center

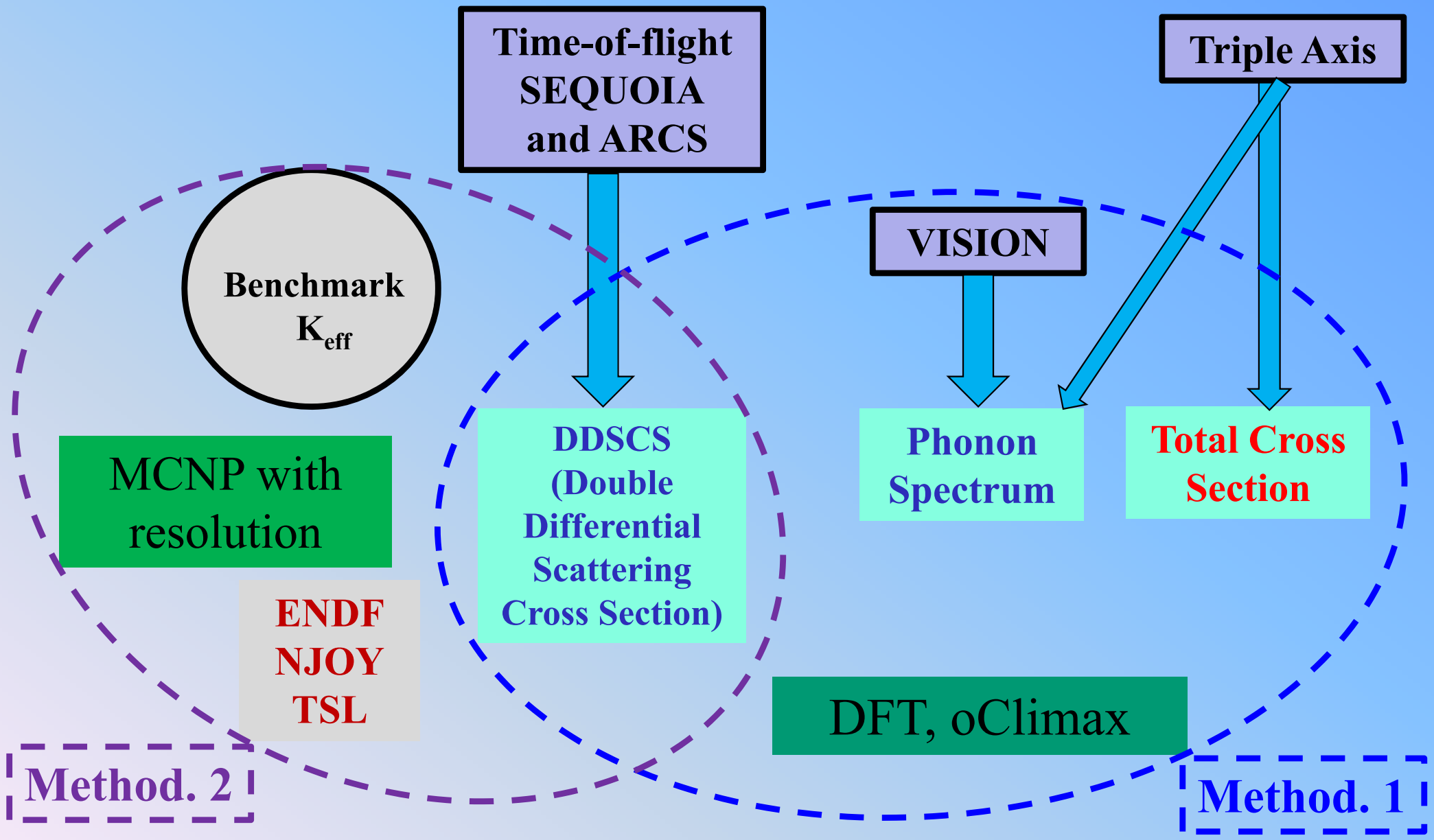
Thermal Scattering Overview

- 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,

- 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.**

Thermal Scattering Experimental Needs



Rensselaer

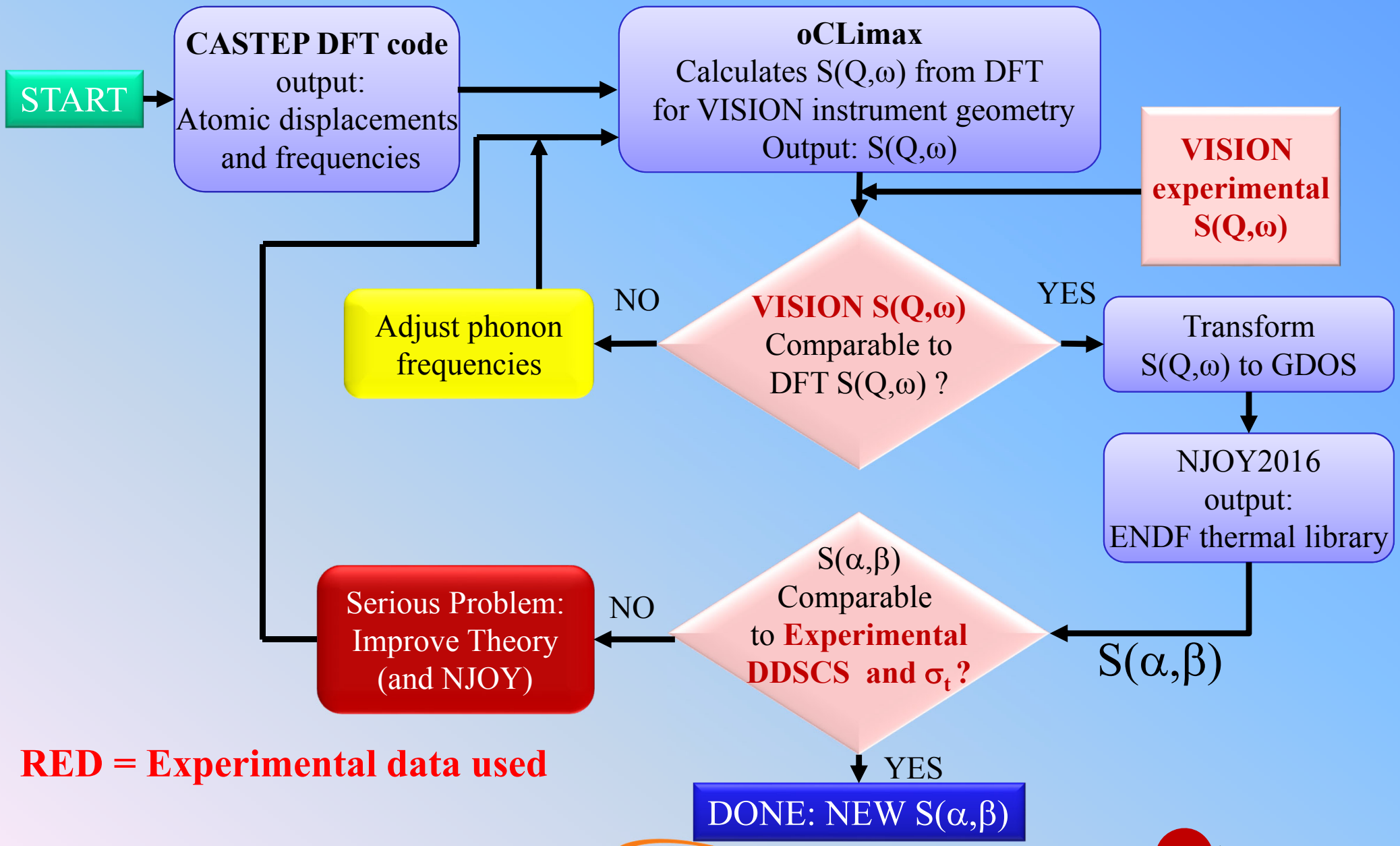
NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

linac The Gaerttner LINAC Center

Completed Experiments

Moderators	SEQUOIA (Ω: 3-58^0 in 1^0 increments)	ARCS (Ω: 3-125^0 in 1^0 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

Thermal scattering – evaluation methodology



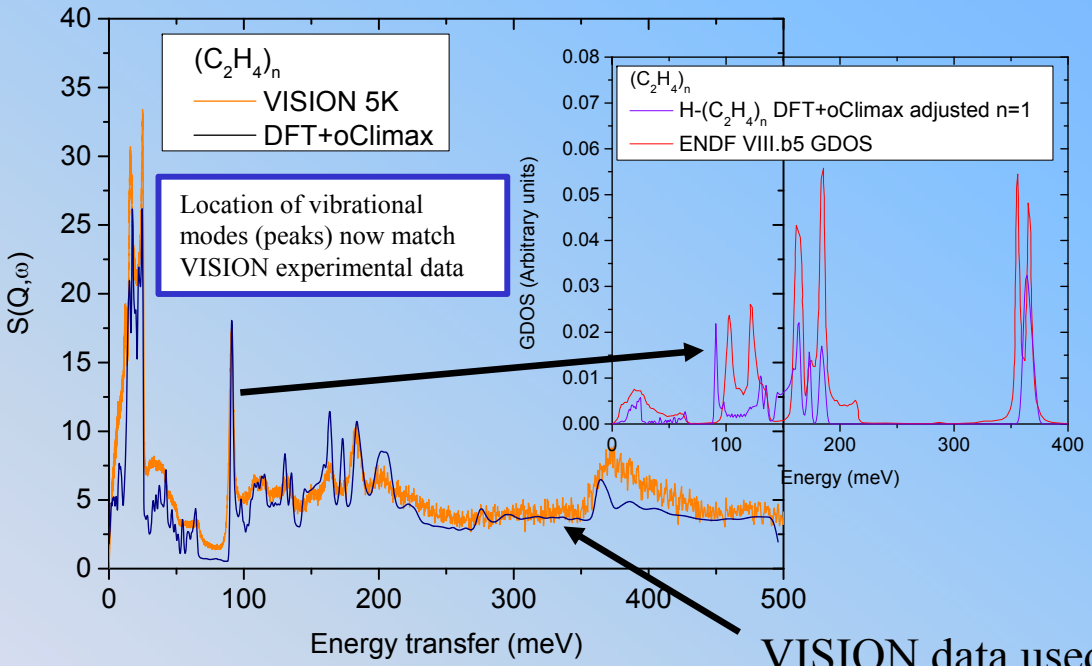
RED = Experimental data used

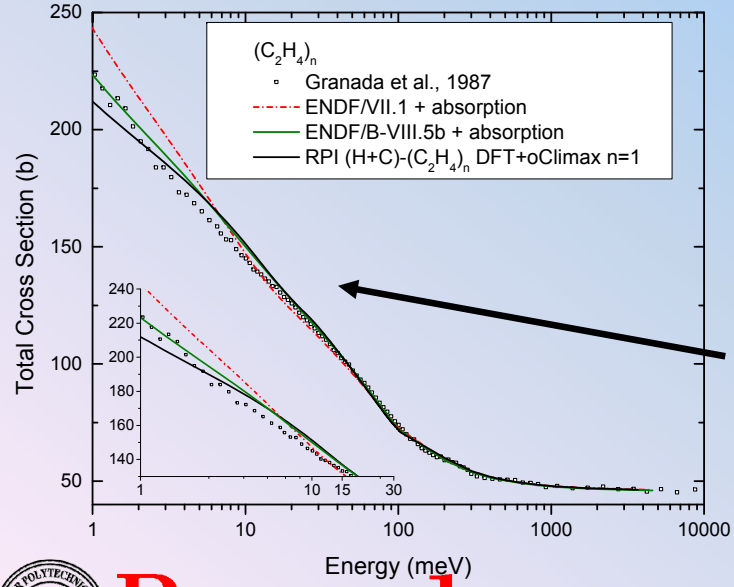
Rensselaer

NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

linac The Gaerttner LINAC Center

Polyethylene Experimental Data and Evaluation

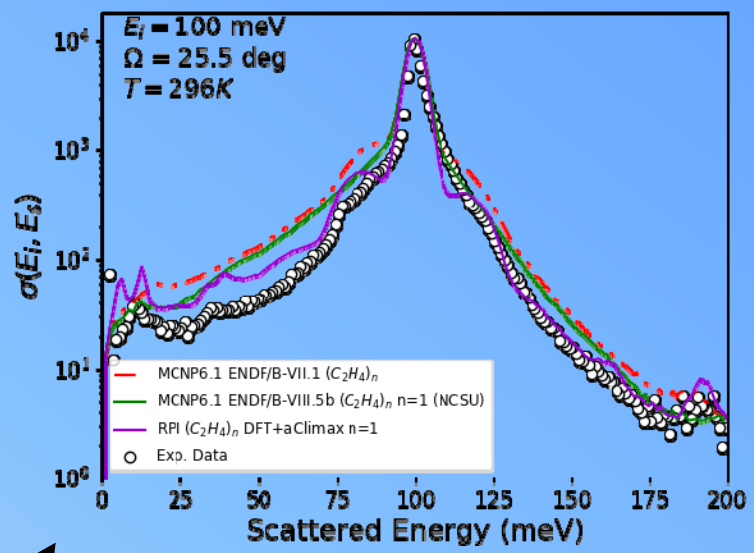


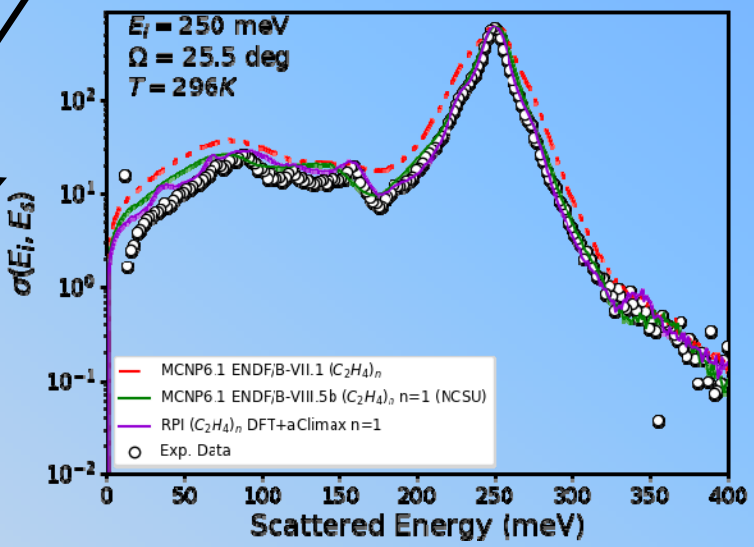


VISION data used to validate and adjust the evaluation

Experimental data used for validation:

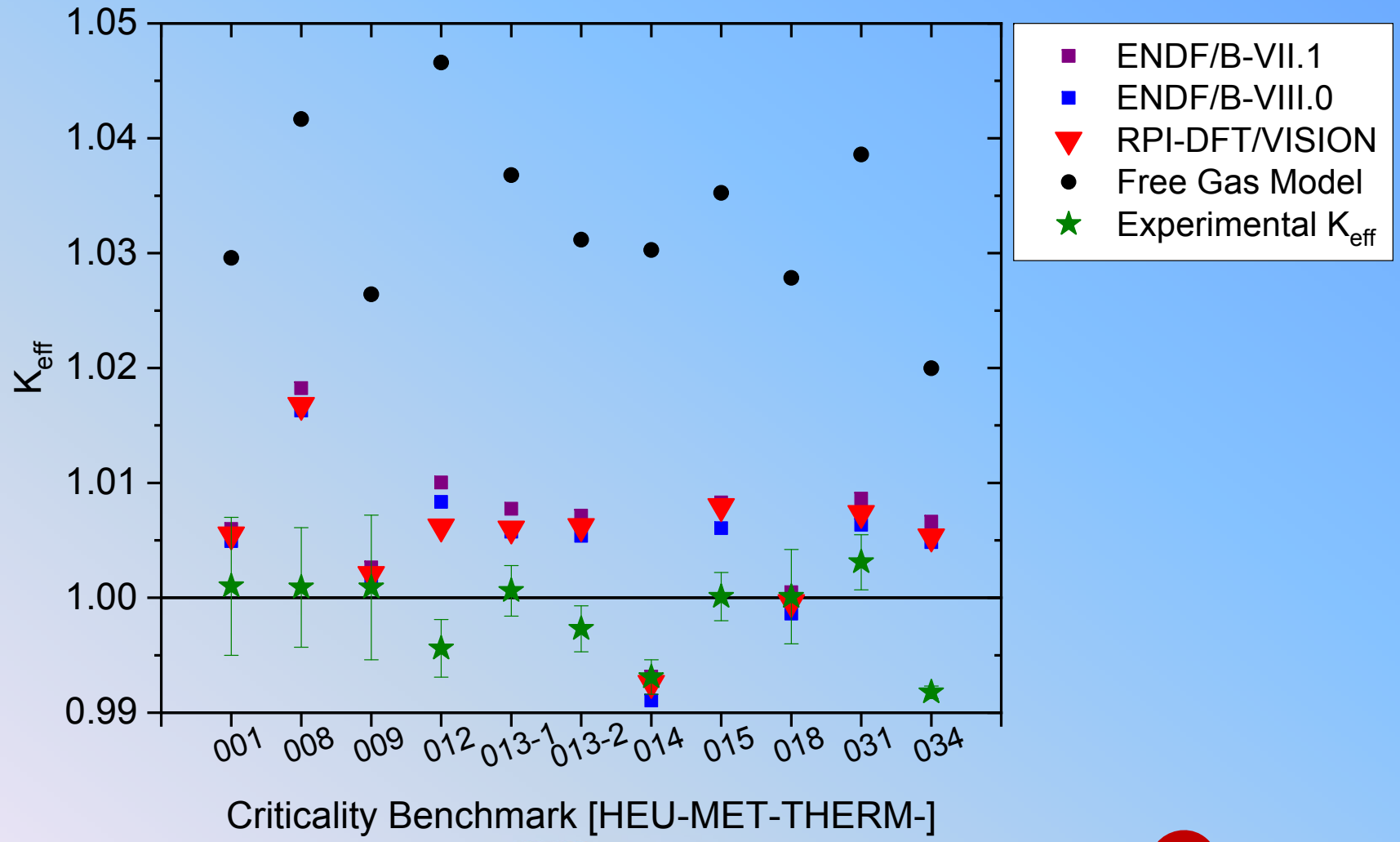
- Double differential scattering
- Total cross section from the literature



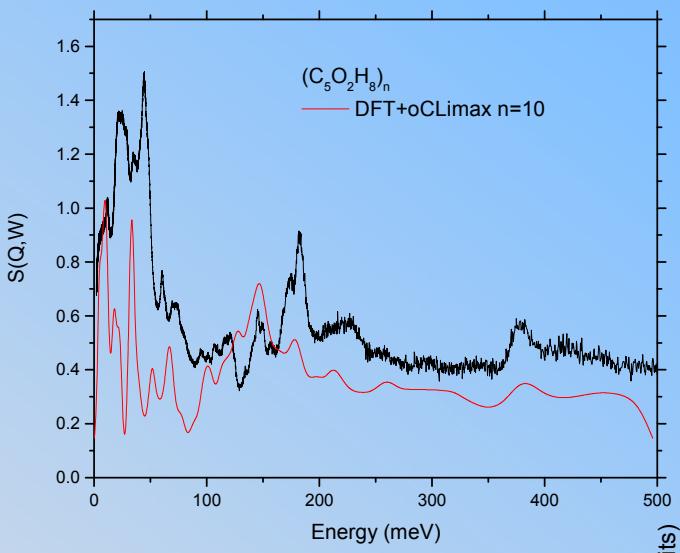


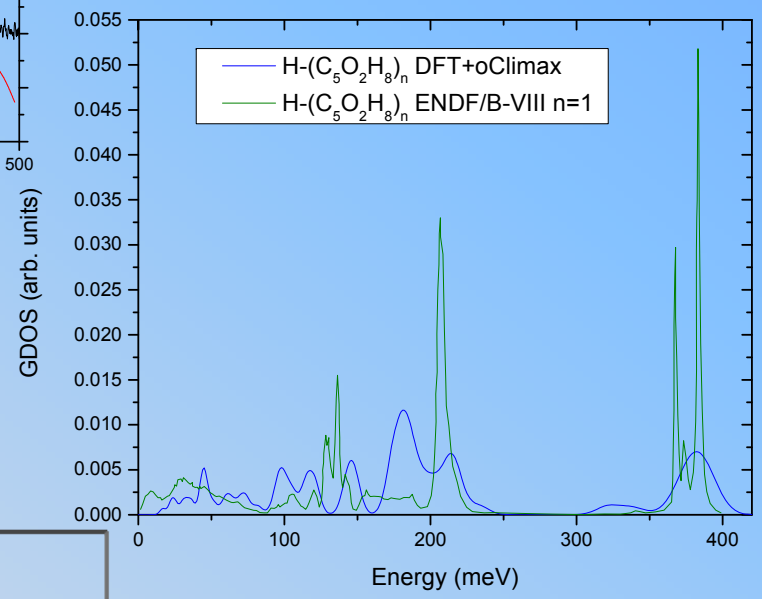
Polyethylene Criticality Benchmarks

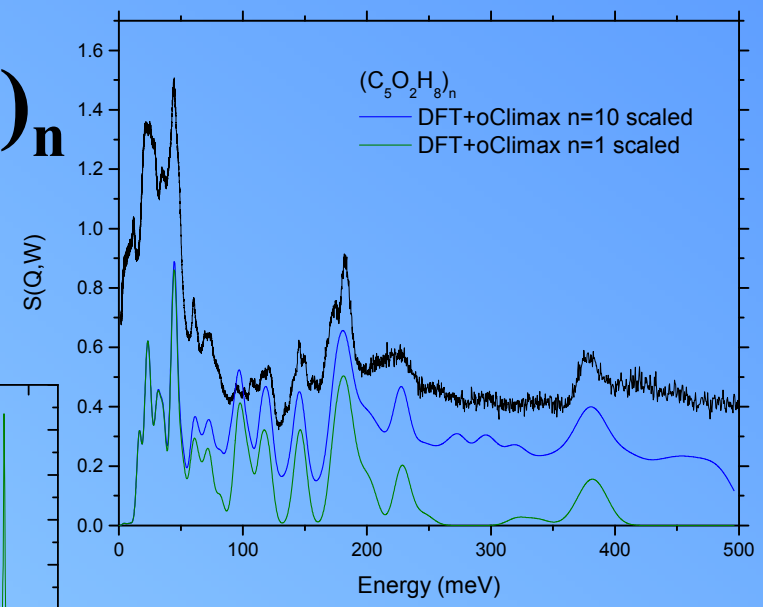
- The new RPI evaluation and the ENDF/B-VIII.0 give similar results.
- There are some discrepancies between the benchmarks and simulation.

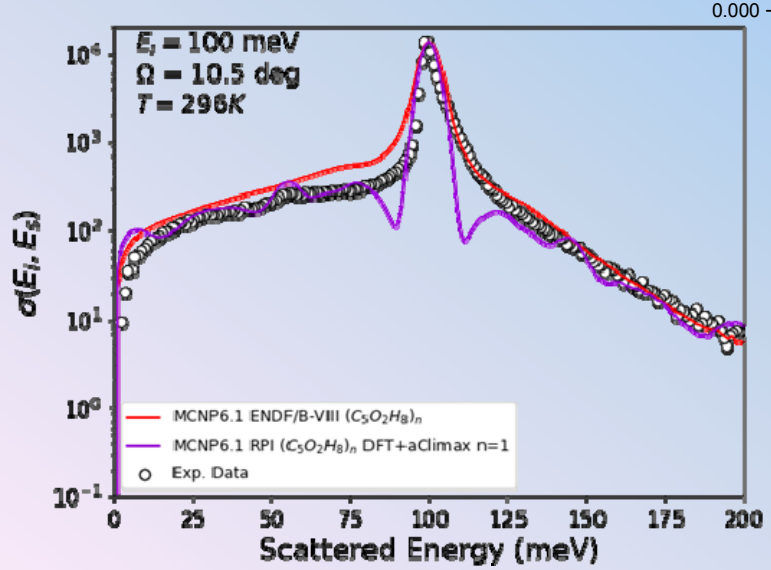


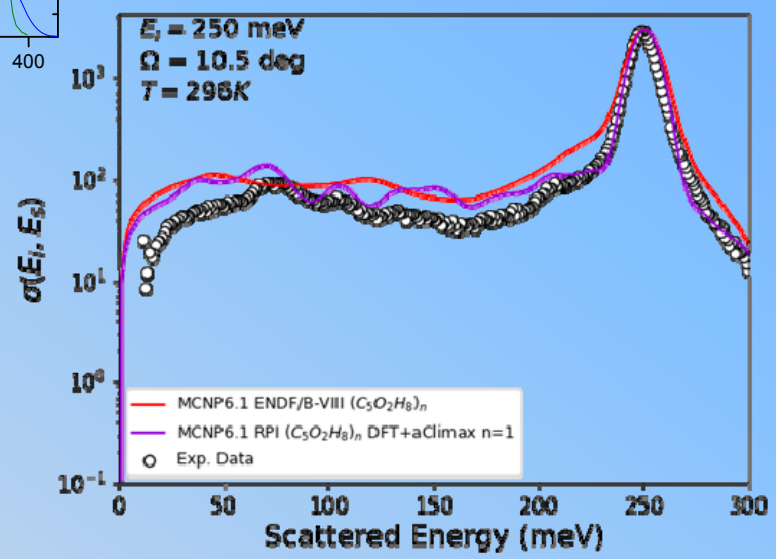
Lucite $(C_5O_2H_8)_n$











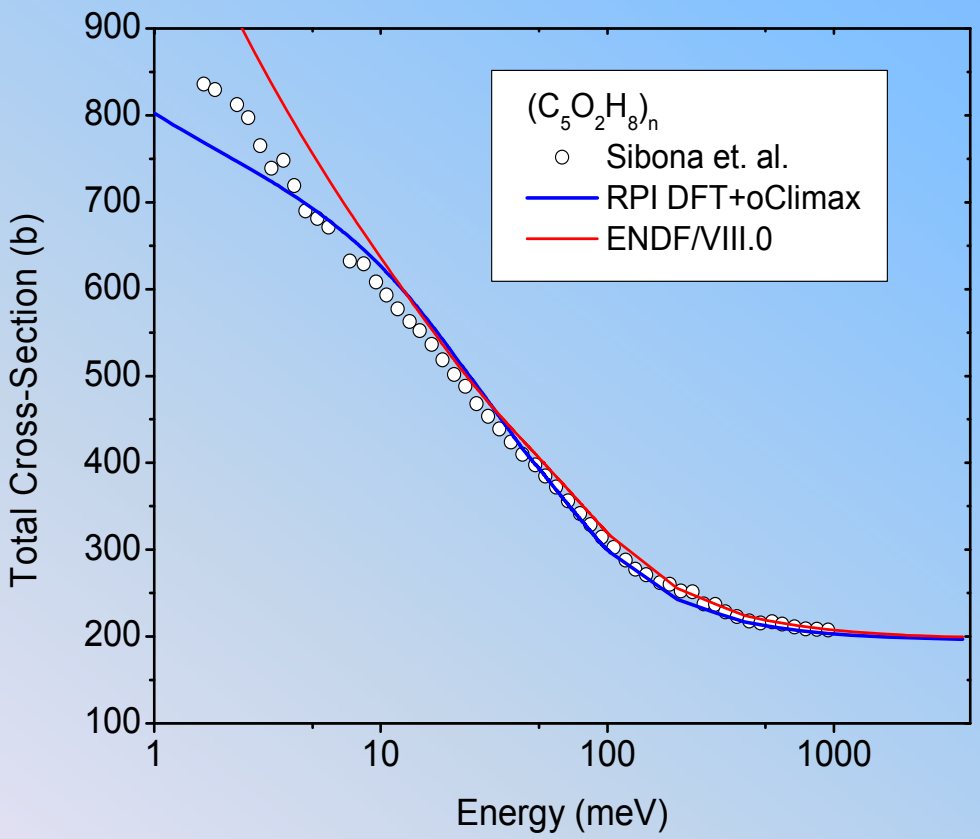
Rensselaer

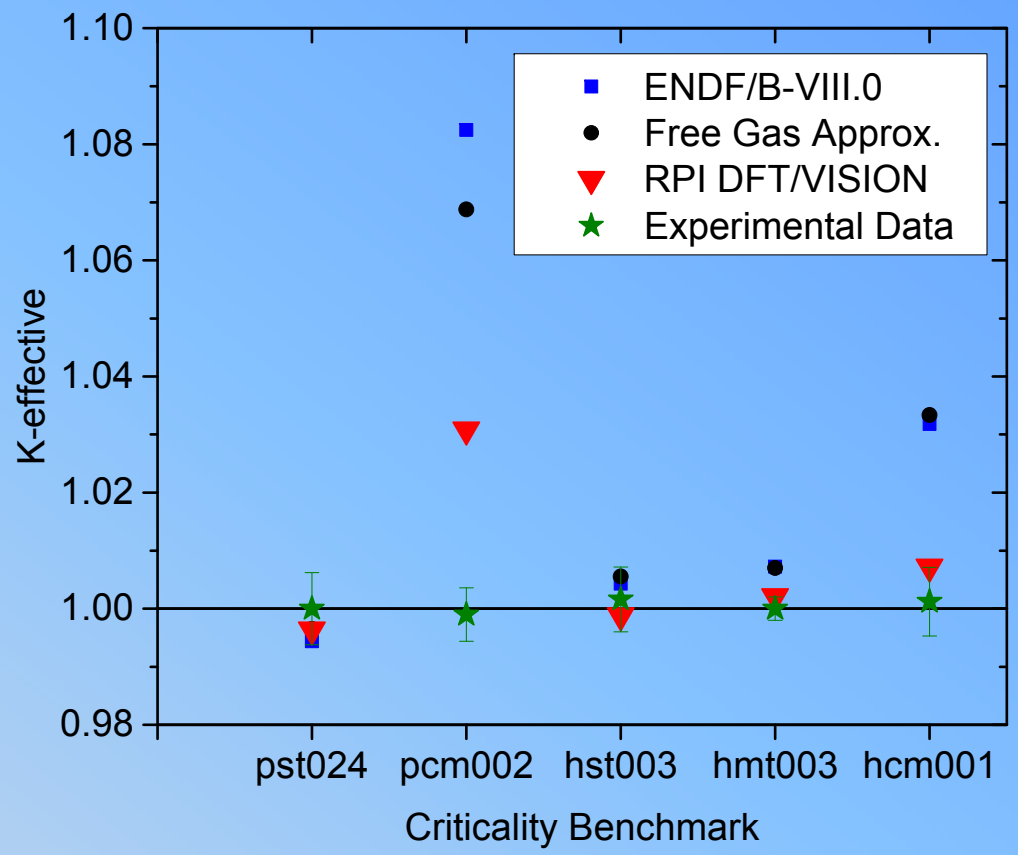
NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

linac The Gaerttner LINAC Center

Lucite $(C_5O_2H_8)_n$

Total cross section and benchmarks





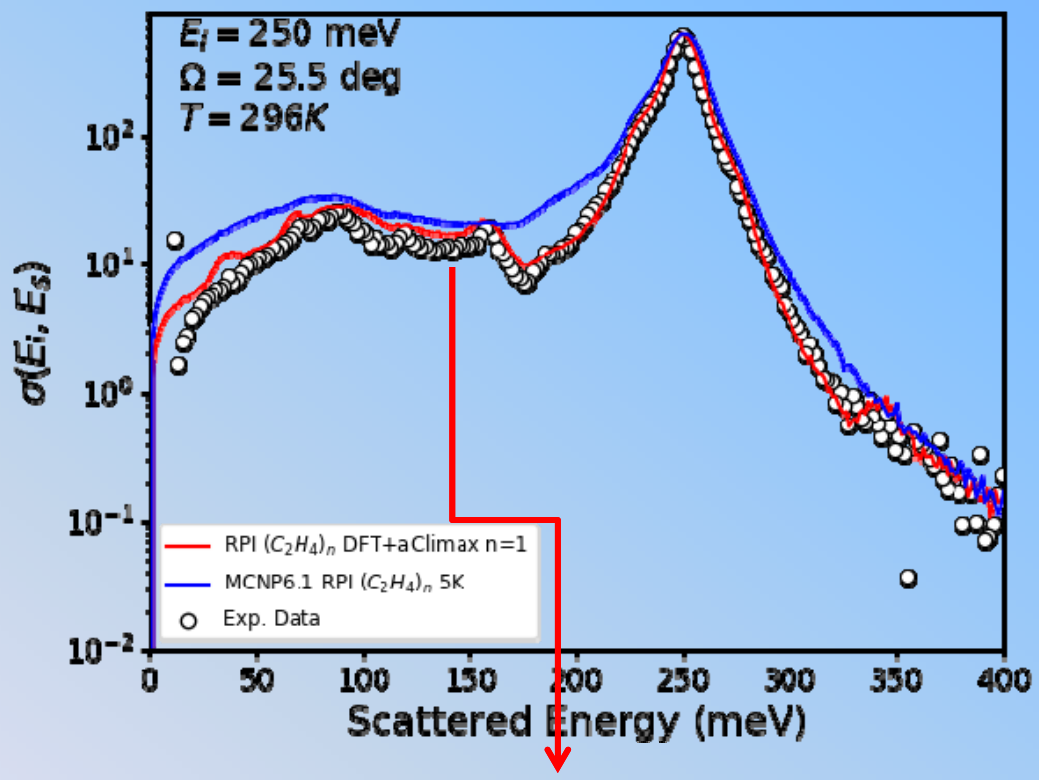
- RPI library represents a clear improvement to K-effective.
- ENDF/B-VIII.0 is similar to free gas treatment.

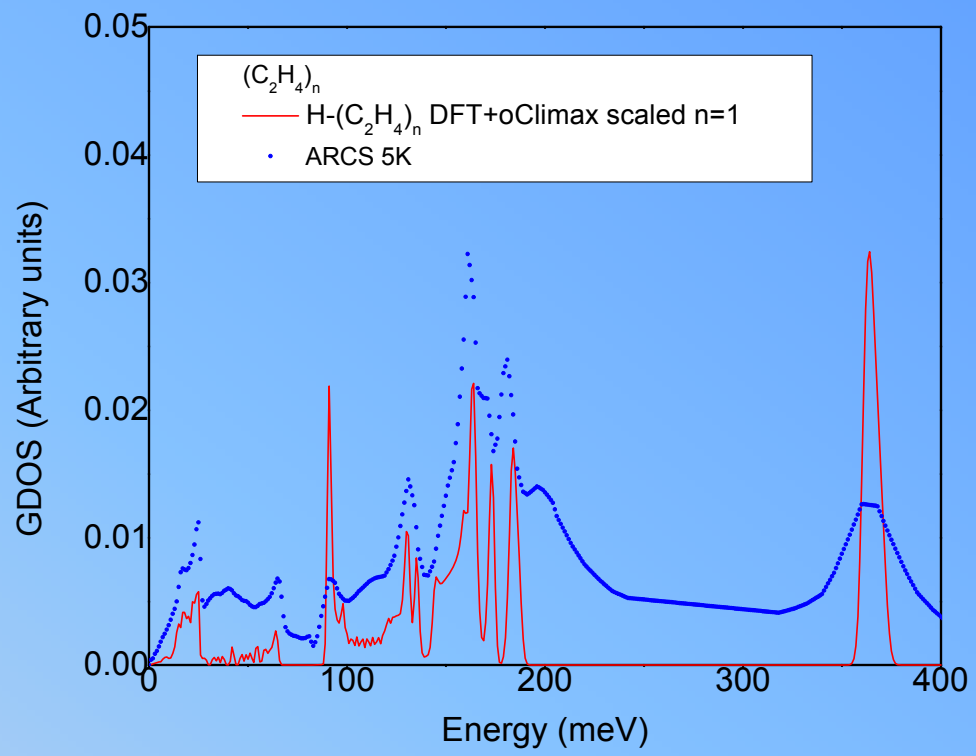
Rensselaer

NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

linac The Gaerttner LINAC Center

Possible Phonon Expansion Issues?



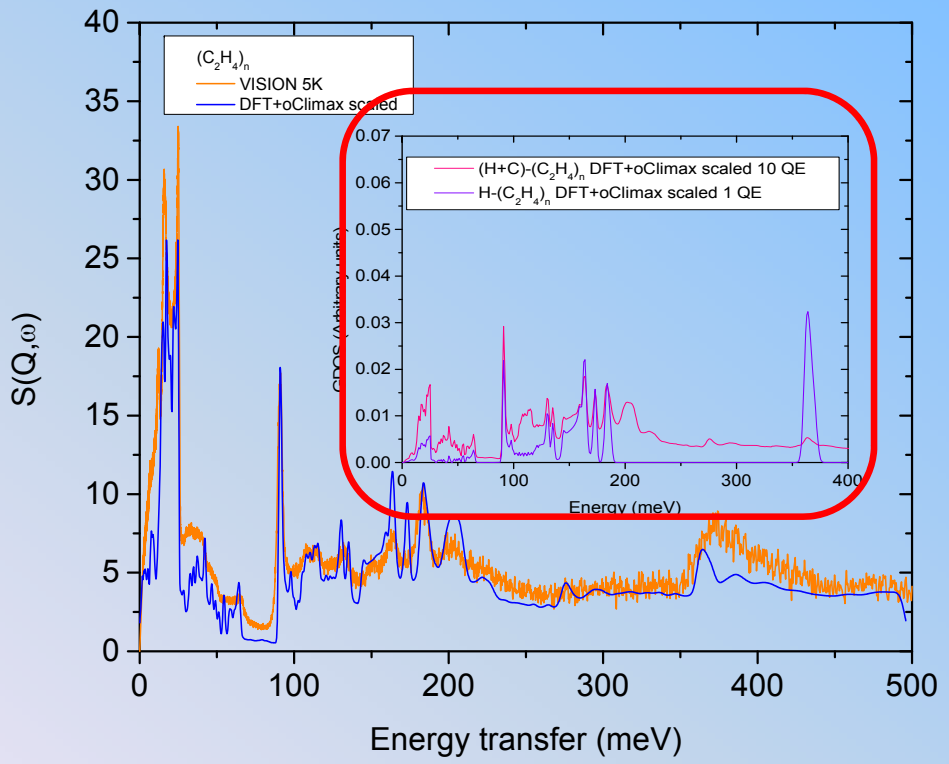


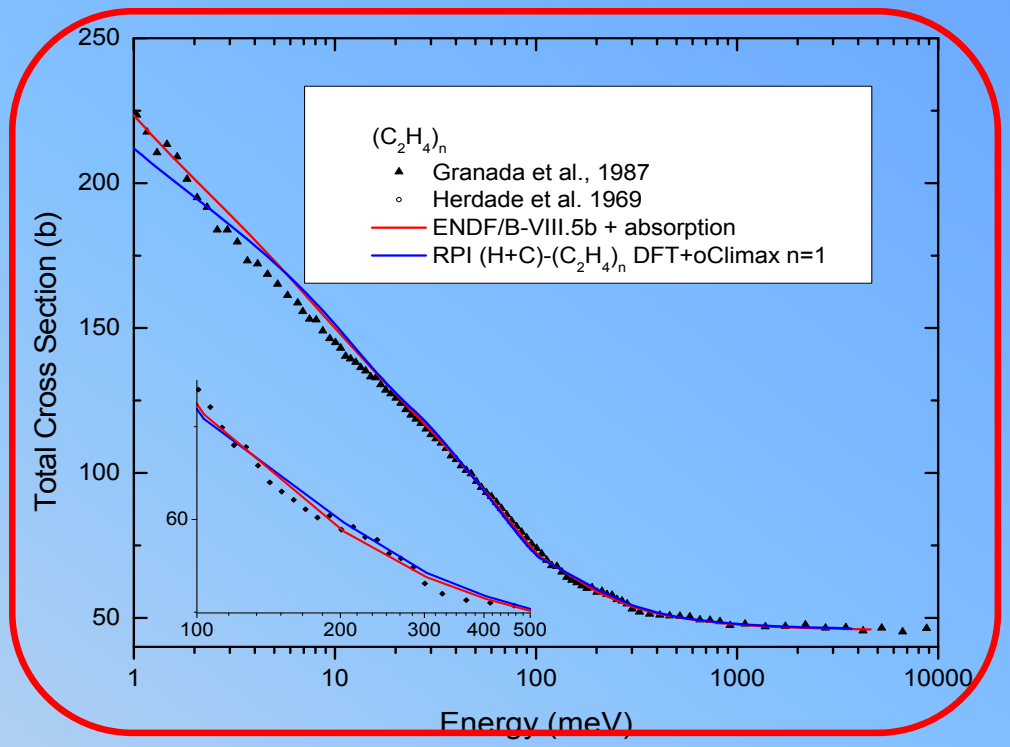
- Phonon expansion:

$$e^{\gamma(t)} = e^{-\alpha\lambda}\sum_{n=0}^{\infty}\frac{1}{n!}\left[P(\beta)e^{i\beta t}e^{-\beta/2}d\beta\right]^{n}$$

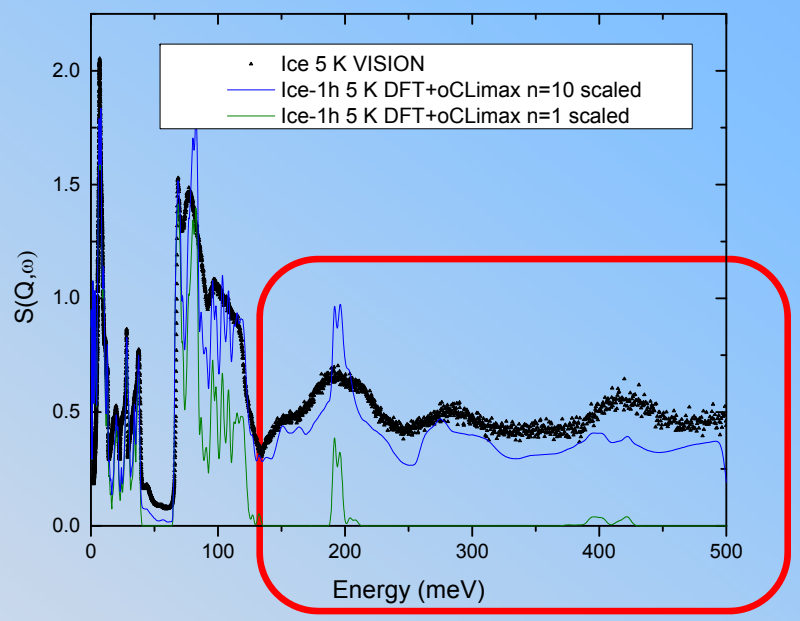
$$S(\alpha,\beta) = e^{-\alpha\lambda}\sum_{n=0}^{\infty}\frac{1}{n!}\alpha^{n}\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\beta t}\left[\int_{-\infty}^{\infty}P(\beta')e^{i\beta' t}e^{-\beta'/2}d\beta'\right]^{n}dt$$

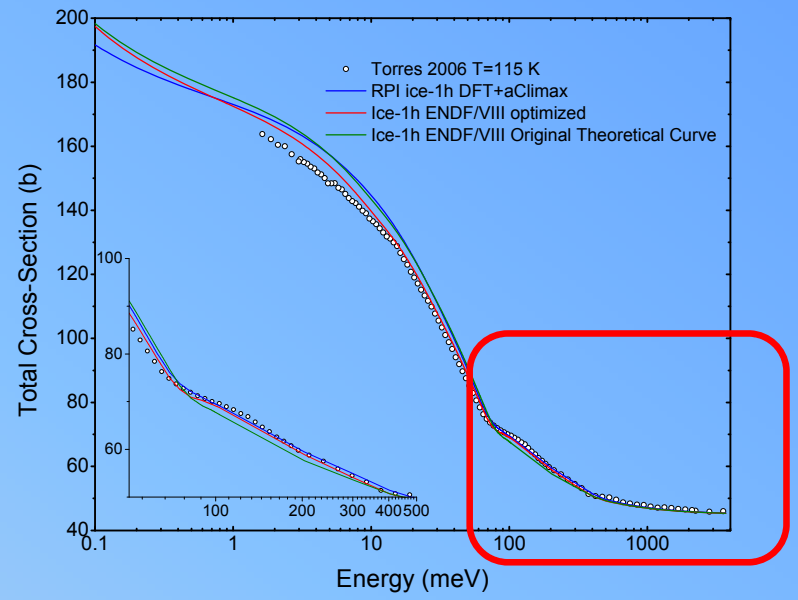
Possible Phonon Expansion Issues?

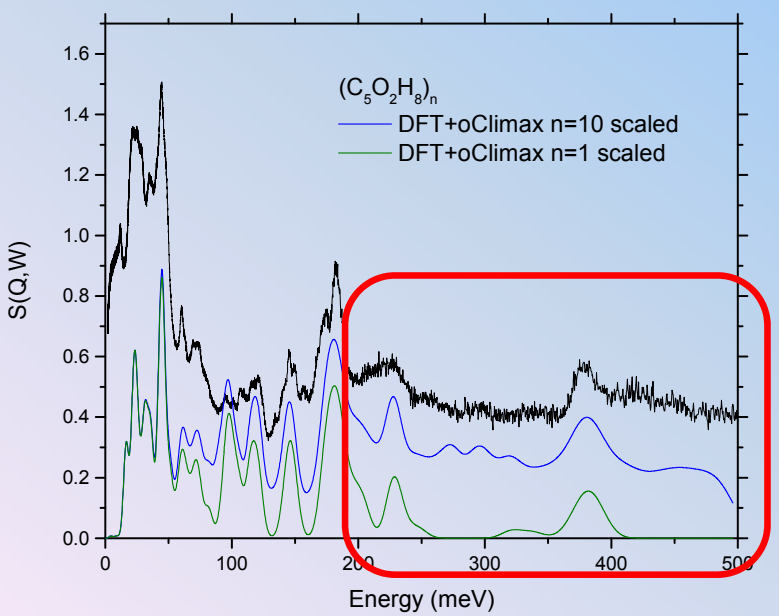


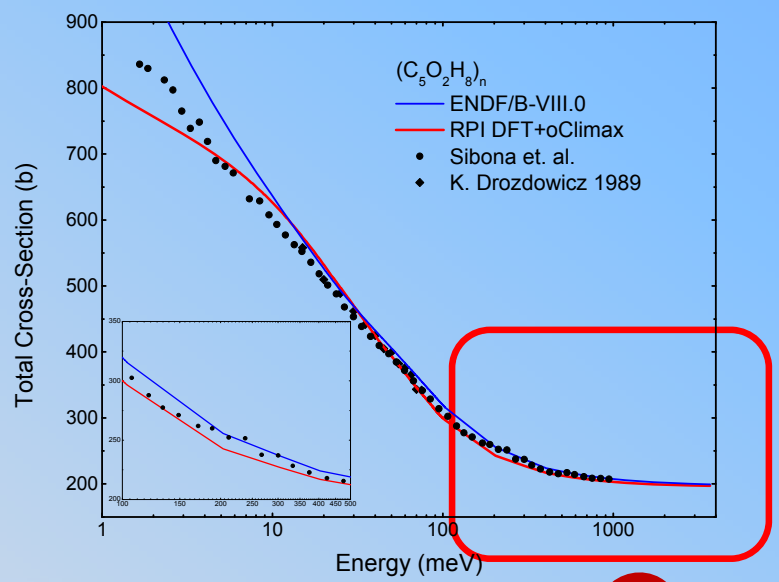


Possible Phonon Expansion Issues?









Questions?

Supplemental Slide