

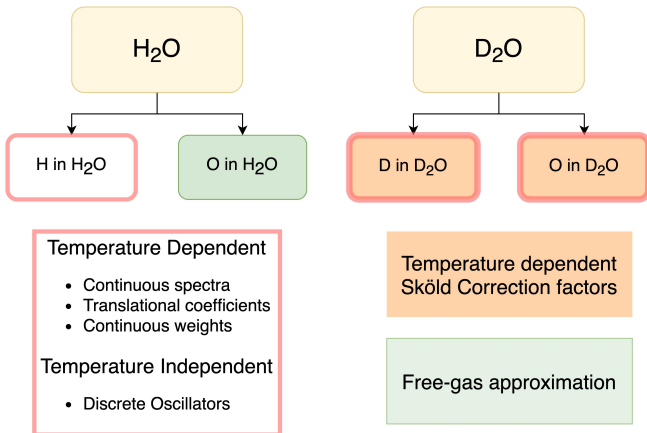
# Thermal Neutron Scattering Effects of Oxygen Bound in Light Water

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# Current State of Water Thermal Scattering Data



# Sköld Correction

$$S(\alpha, \beta) = S_{inc}(\alpha, \beta) + S_{coh}(\alpha, \beta)$$

Typically neglect coherent effects

LEAPR allows for coherent effects to be approximated using Sköld correction:

$$S_{coh}(\alpha, \beta) = S_{inc}\left(\frac{\alpha}{\tilde{S}(Q)}, \beta\right) \times \tilde{S}(Q)$$

$\tilde{S}(Q)$  = Sköld correction factors  
(different for hydrogen vs. oxygen)

## Improvements Made

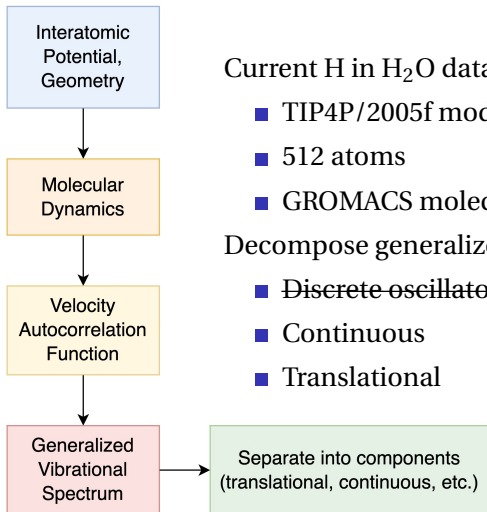
Since O in H<sub>2</sub>O is currently treated as a free gas, the importance of its vibrational spectra is not known.

The D<sub>2</sub>O evaluation uses the Sköld correction, but H<sub>2</sub>O does not

- Generate O in H<sub>2</sub>O vibrational spectrum
- Obtain Sköld correction factors for coherence

Evaluations developed in this project were made using same methods as used for existing D<sub>2</sub>O and H in H<sub>2</sub>O evaluations

# H in H<sub>2</sub>O Evaluation Generation



Current H in H<sub>2</sub>O data generated using

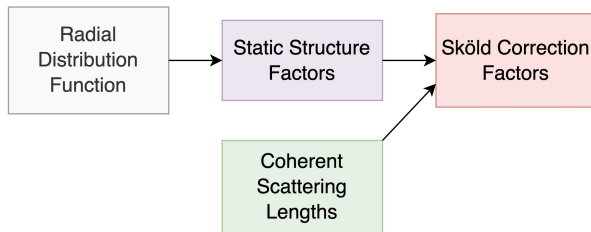
- TIP4P/2005f model
- 512 atoms
- GROMACS molecular dynamics code

Decompose generalized VDOS into

- Discrete oscillators
- Continuous
- Translational

*Not using discrete oscillators for current work*

# Generating Sköld Correction Factors for H<sub>2</sub>O



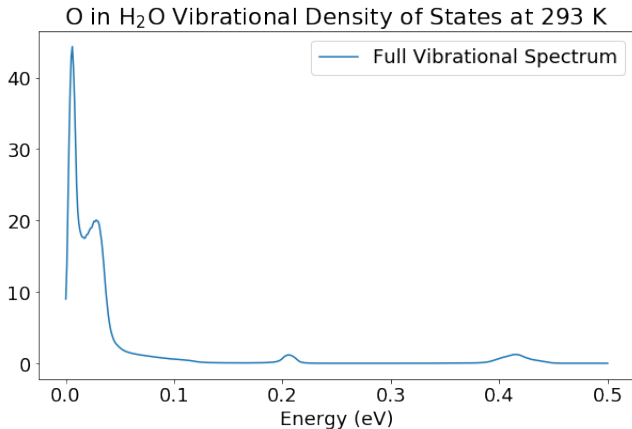
$$S(\alpha, \beta) = S_{inc}(\alpha, \beta) + S_{coh}(\alpha, \beta)$$

$$S_{coh}(\alpha, \beta) = S_{inc}\left(\frac{\alpha}{\tilde{S}(Q)}, \beta\right) \times \tilde{S}(Q)$$

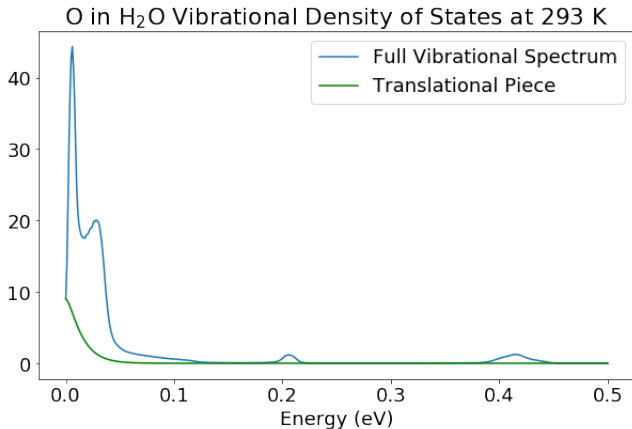
$\tilde{S}(Q)$  = Sköld correction factors

differ for hydrogen vs. oxygen

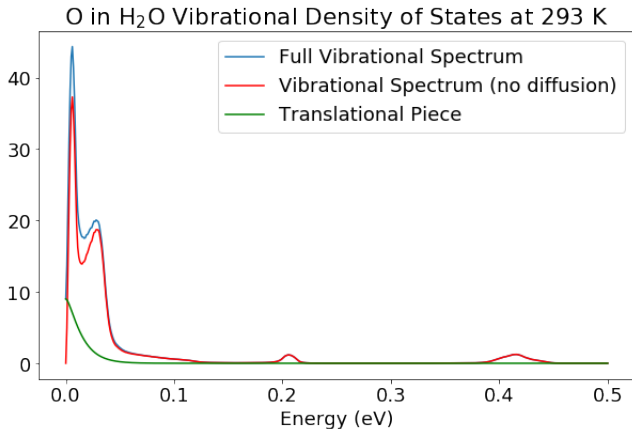
# New O in H<sub>2</sub>O Vibrational Spectrum



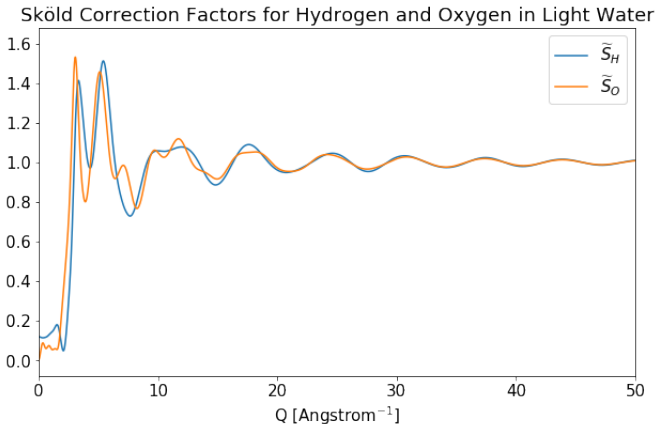
# New O in H<sub>2</sub>O Vibrational Spectrum



# New O in H<sub>2</sub>O Vibrational Spectrum

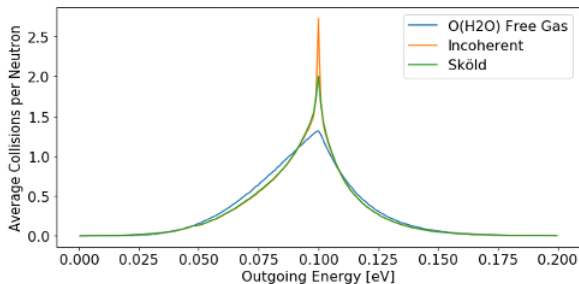


# Sköld Correction Factors for H<sub>2</sub>O



# Outgoing Neutron Energy Distribution, O in H<sub>2</sub>O

Incoming neutron energy 0.1 eV



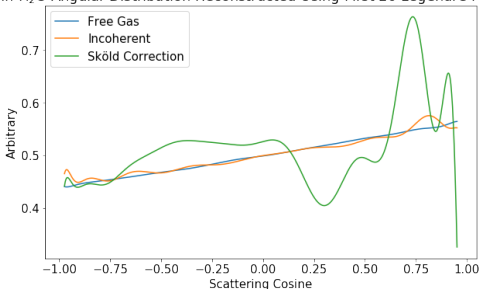
Modified OpenMC to tally single collision event on O in H<sub>2</sub>O

Addition of O in H<sub>2</sub>O frequency spectrum strongly affects outgoing energy distribution

# Outgoing Neutron Angular Distribution, O in H<sub>2</sub>O

Incoming neutron energy 0.1 eV

O in H<sub>2</sub>O Angular Distribution Reconstructed Using First 20 Legendre Moments



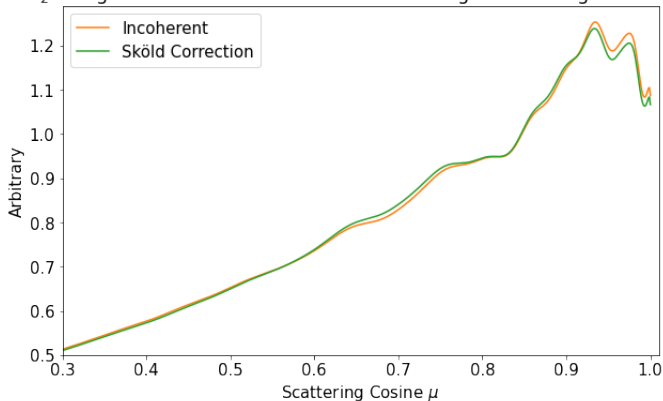
$$S_{coh}(\alpha, \beta) = S_{inc}\left(\frac{\alpha}{\tilde{S}(Q)}, \beta\right) \times \tilde{S}(Q)$$

Since Sköld correction scales the  $\alpha$  argument, it is expected to have a large effect on the angular distribution

# Outgoing Neutron Angular Distribution, H in H<sub>2</sub>O

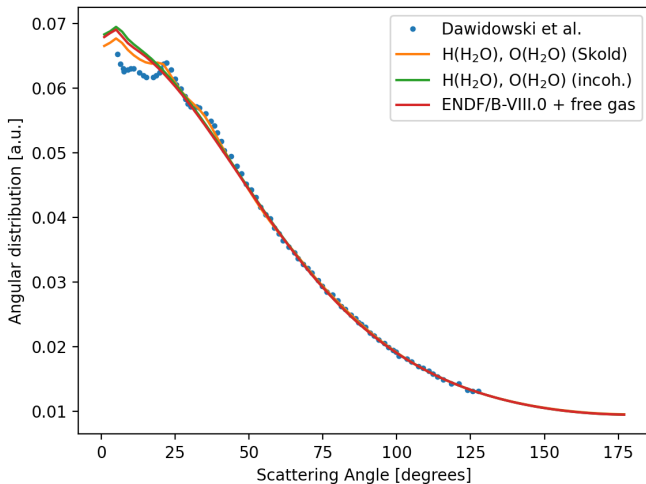
Incoming neutron energy 0.1 eV

H in H<sub>2</sub>O Angular Distribution Reconstructed Using First 80 Legendre Moments



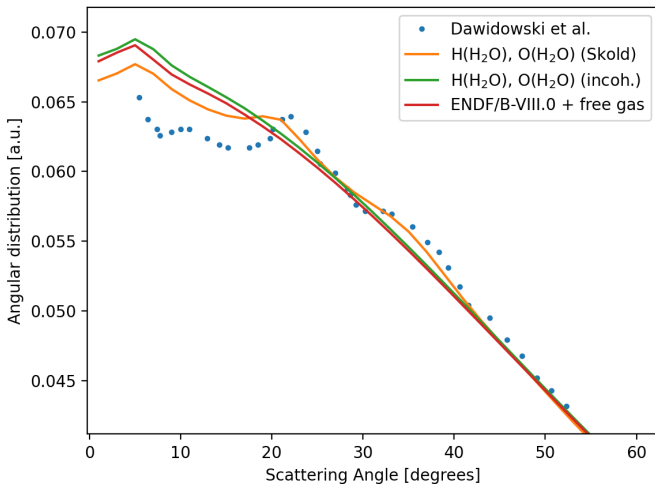
# Comparison with Experiment

Angular Distribution, Incoming neutron energy 0.1614 eV



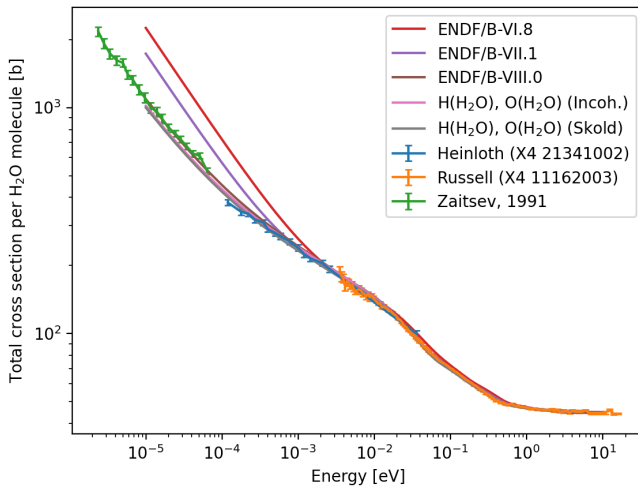
# Comparison with Experiment

Angular Distribution, Incoming neutron energy 0.1614 eV



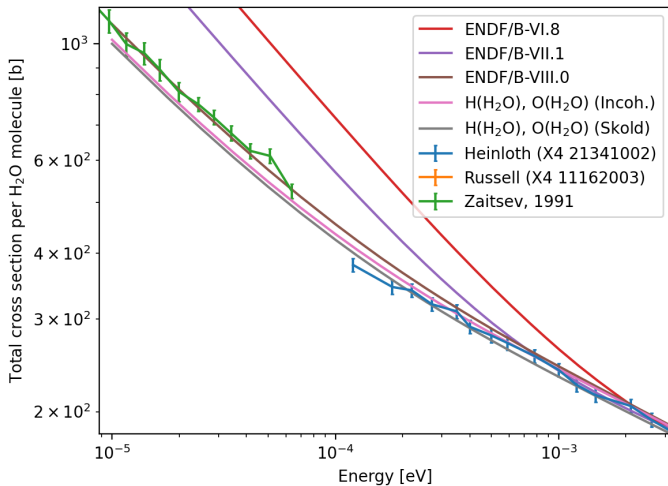
# Comparison with Experiment

## Total Cross Section per H<sub>2</sub>O Molecule



# Comparison with Experiment

## Total Cross Section per H<sub>2</sub>O Molecule



# Conclusion

- Improved thermal scattering evaluation for light water has been developed
  - Created O in H<sub>2</sub>O vibrational spectra
  - Generated Sköld correction factors for H<sub>2</sub>O
- New data creates noticeable shift for oxygen-neutron scattering (both angle and energy)
- Addition of the Sköld correction factors noticeably shifts H<sub>2</sub>O angular distribution to further agree with experiment