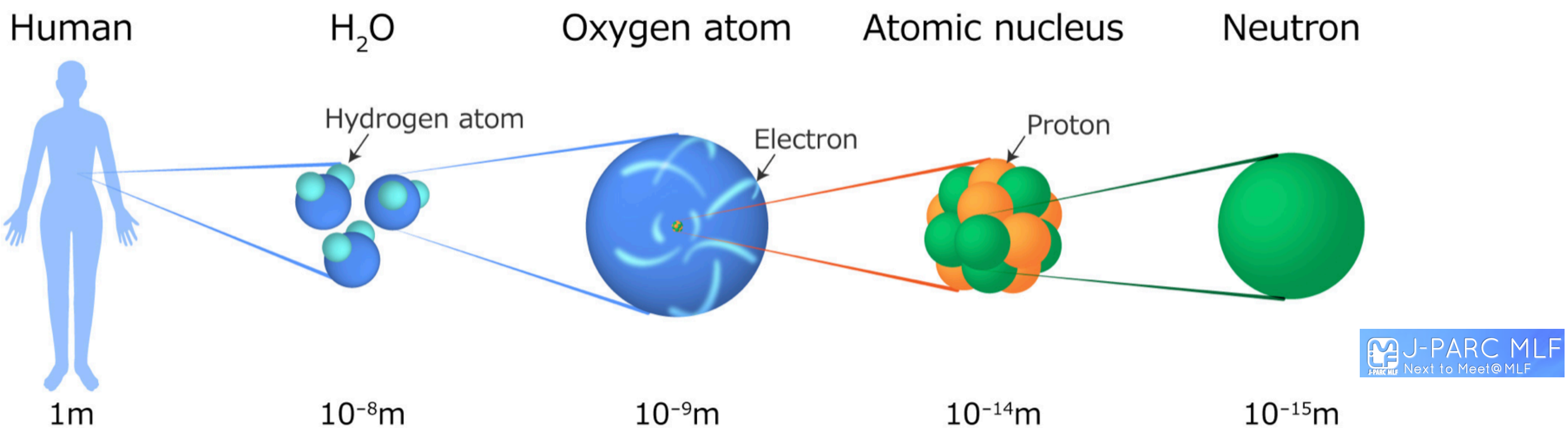
# Using Neutrons for Material Research

WNPPC2023

**Marcella Berg**

**Marcella.Berg@uregina.ca**

# Neutron Scattering



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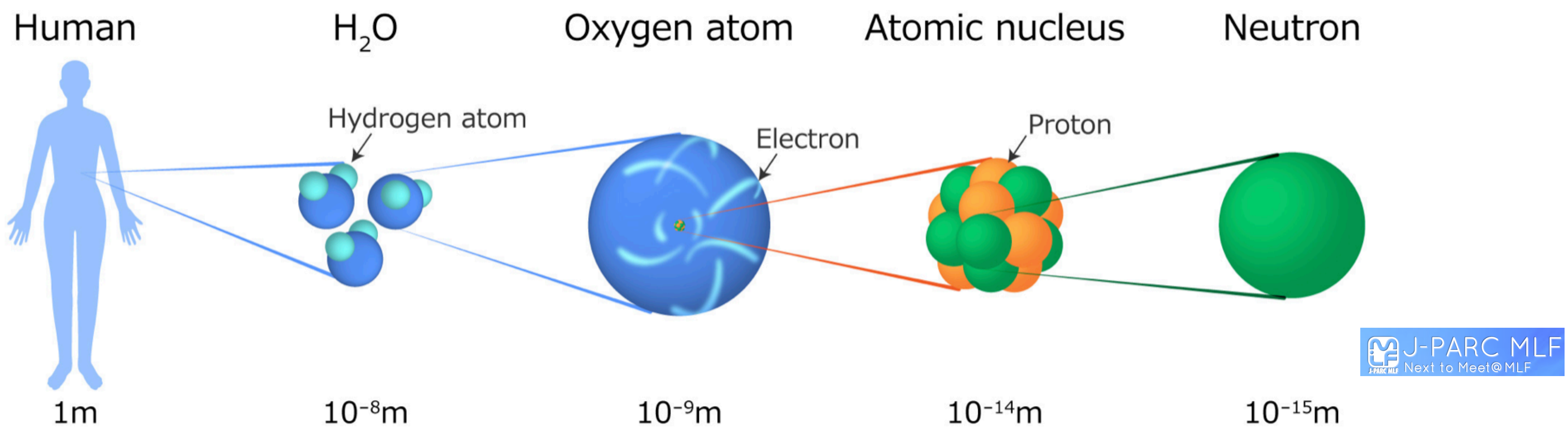


- **Wavelength comparable with interatomic spacings**
- **Kinetic energy comparable with that of atoms in a solid**
- **Interacts with an atom's nucleus, the bulk properties are measured and sample can be contained**
- **Carry no charge**
- **Weak interaction with matter aids interpretation of scattering data**
- **Isotopic sensitivity allows contrast variation**
- **Neutron magnetic moment couples to B, so the neutron “sees” unpaired electron spins**



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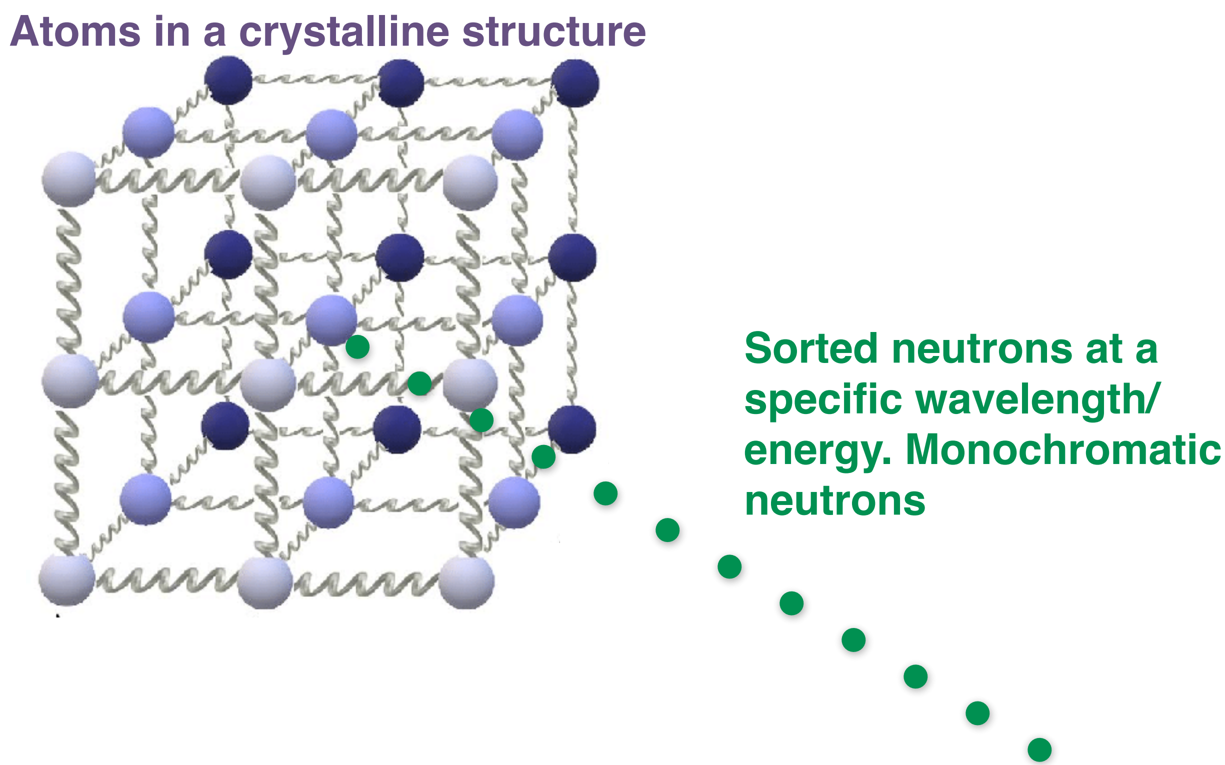
# Neutron Scattering

- Why do Neutron Scattering?
  - Neutrons show you where the atoms are



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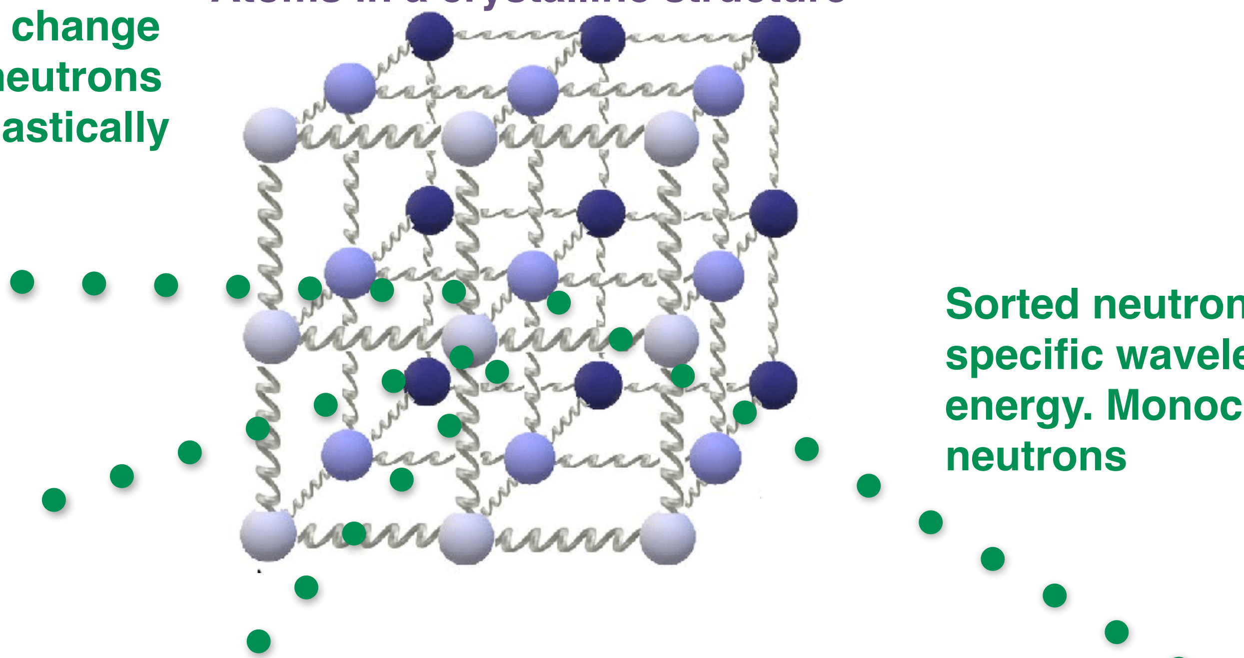

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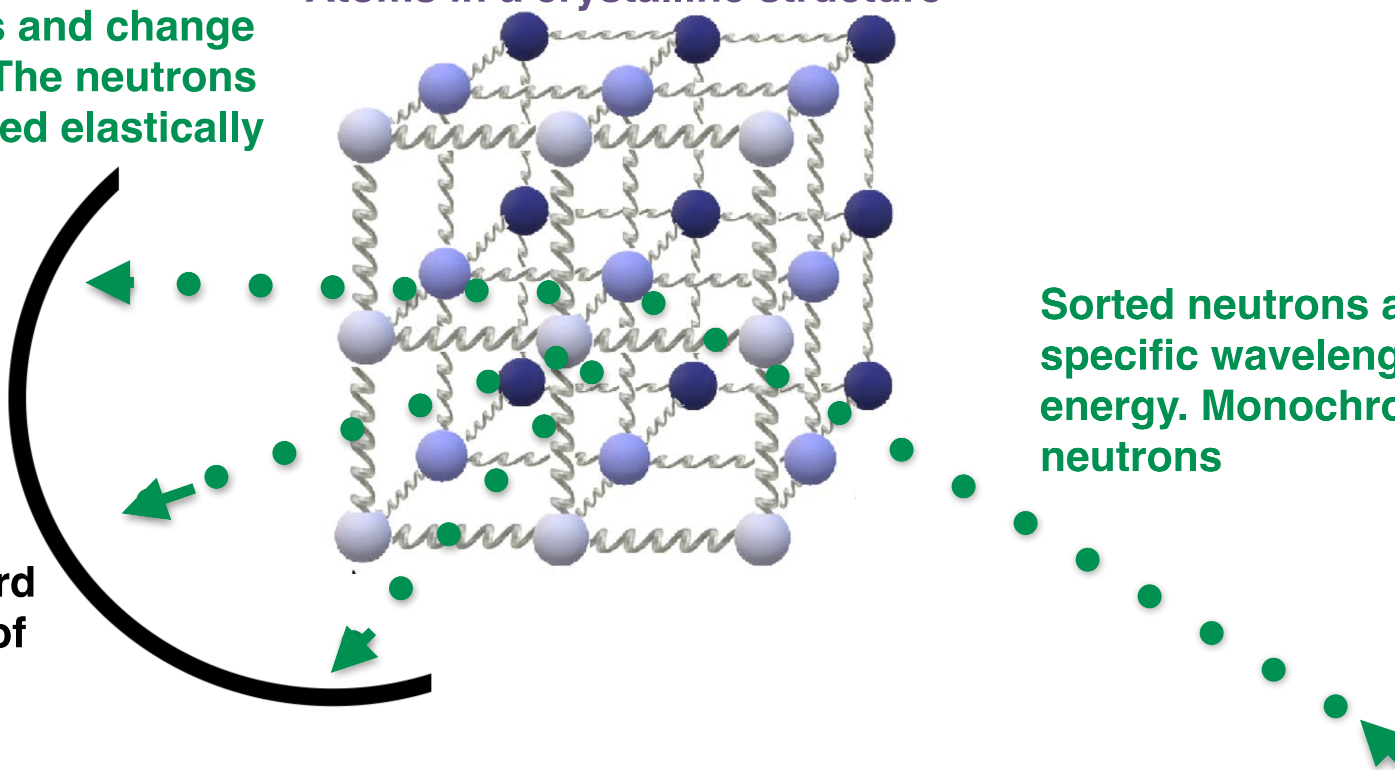




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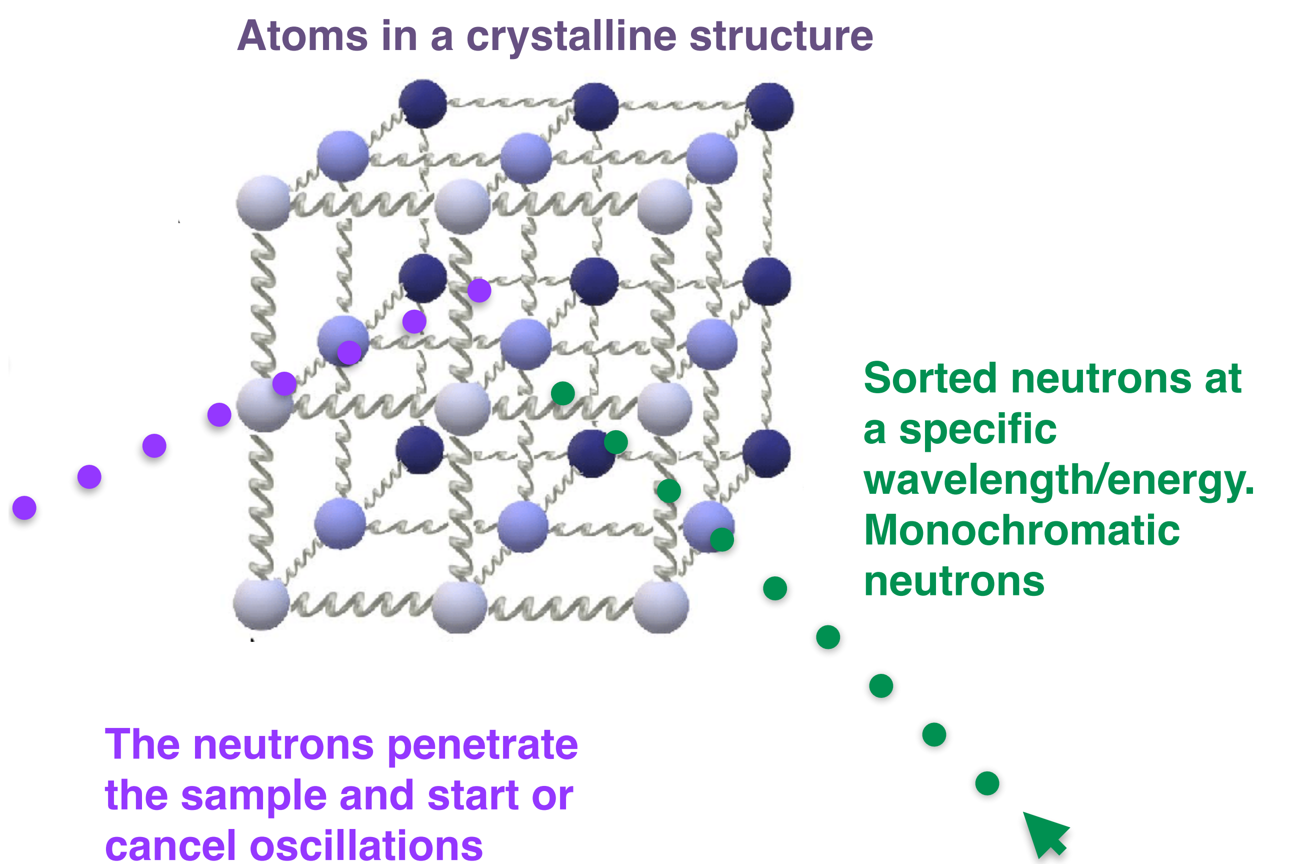

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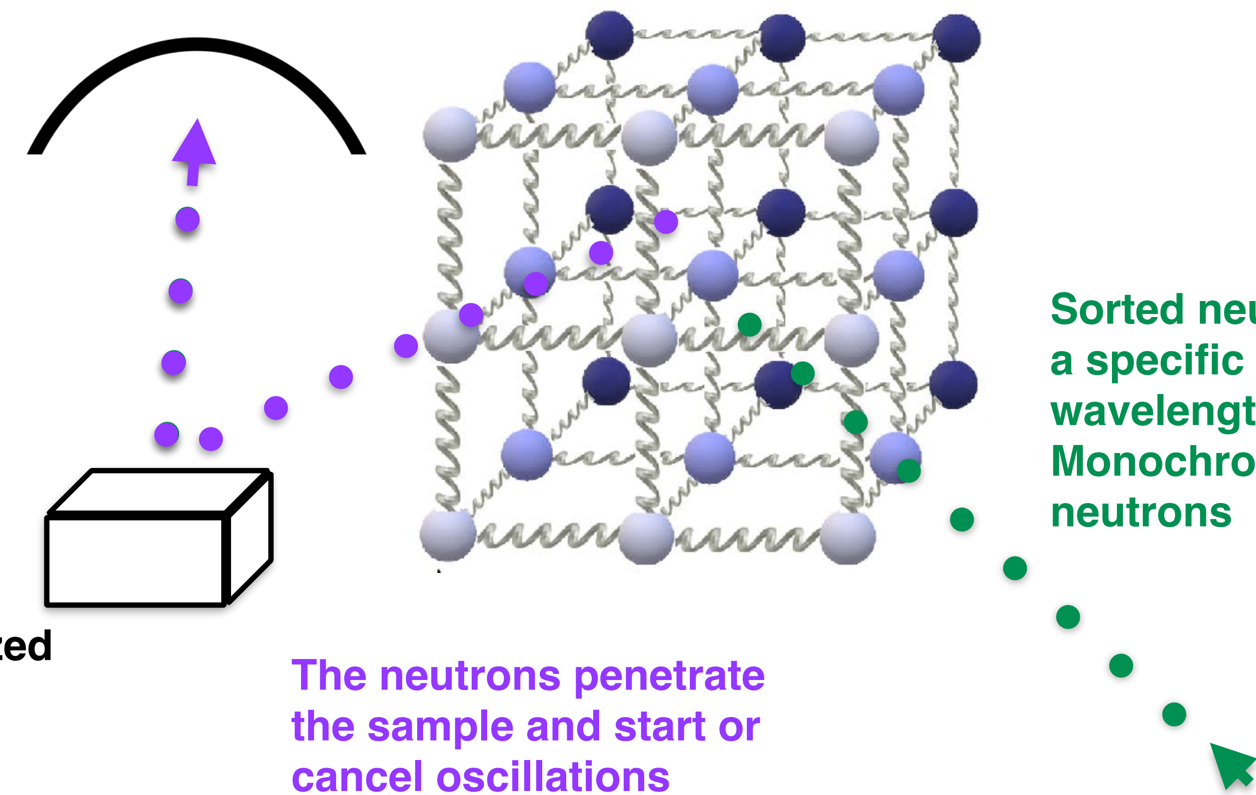
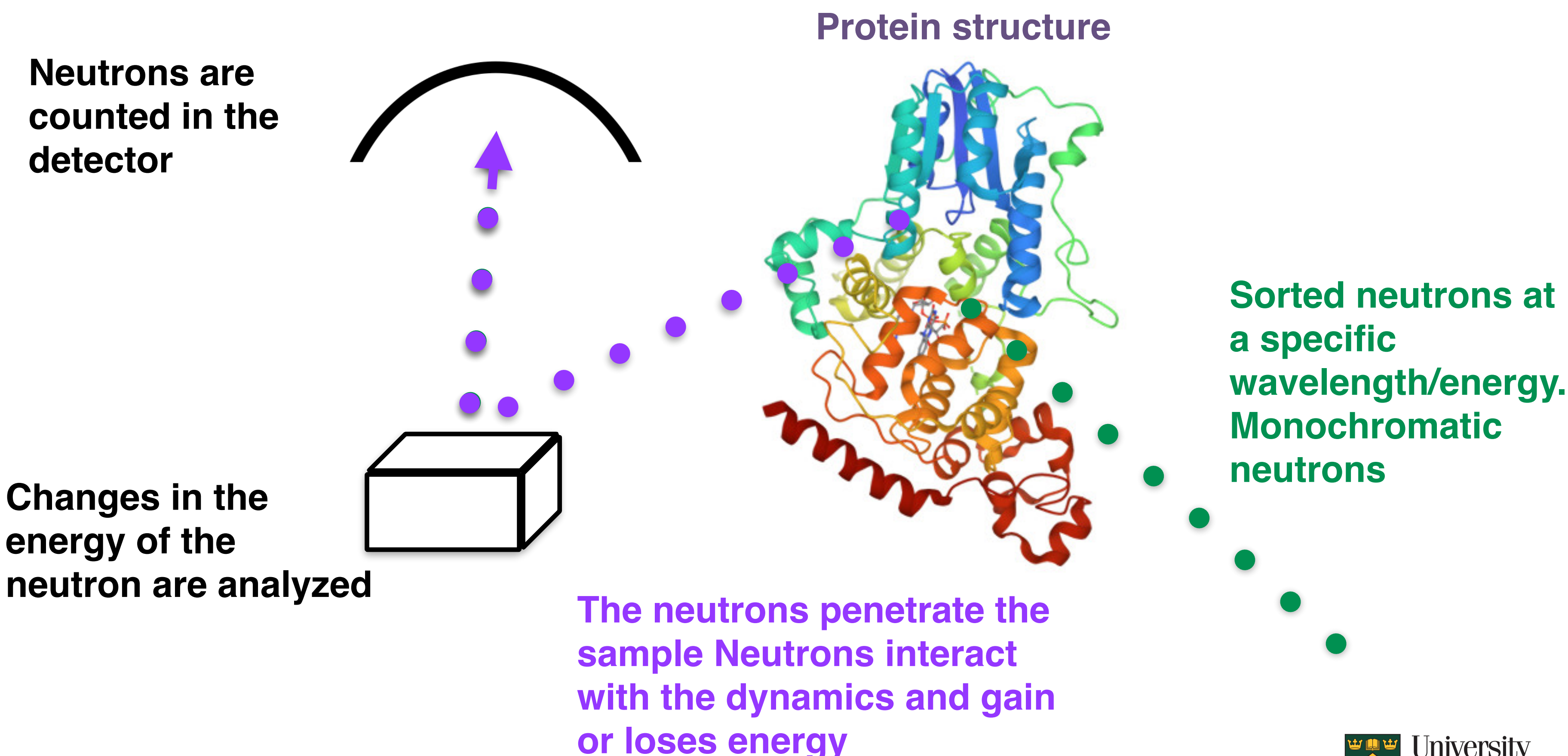


# Neutron Scattering

- It also works with other types of sample



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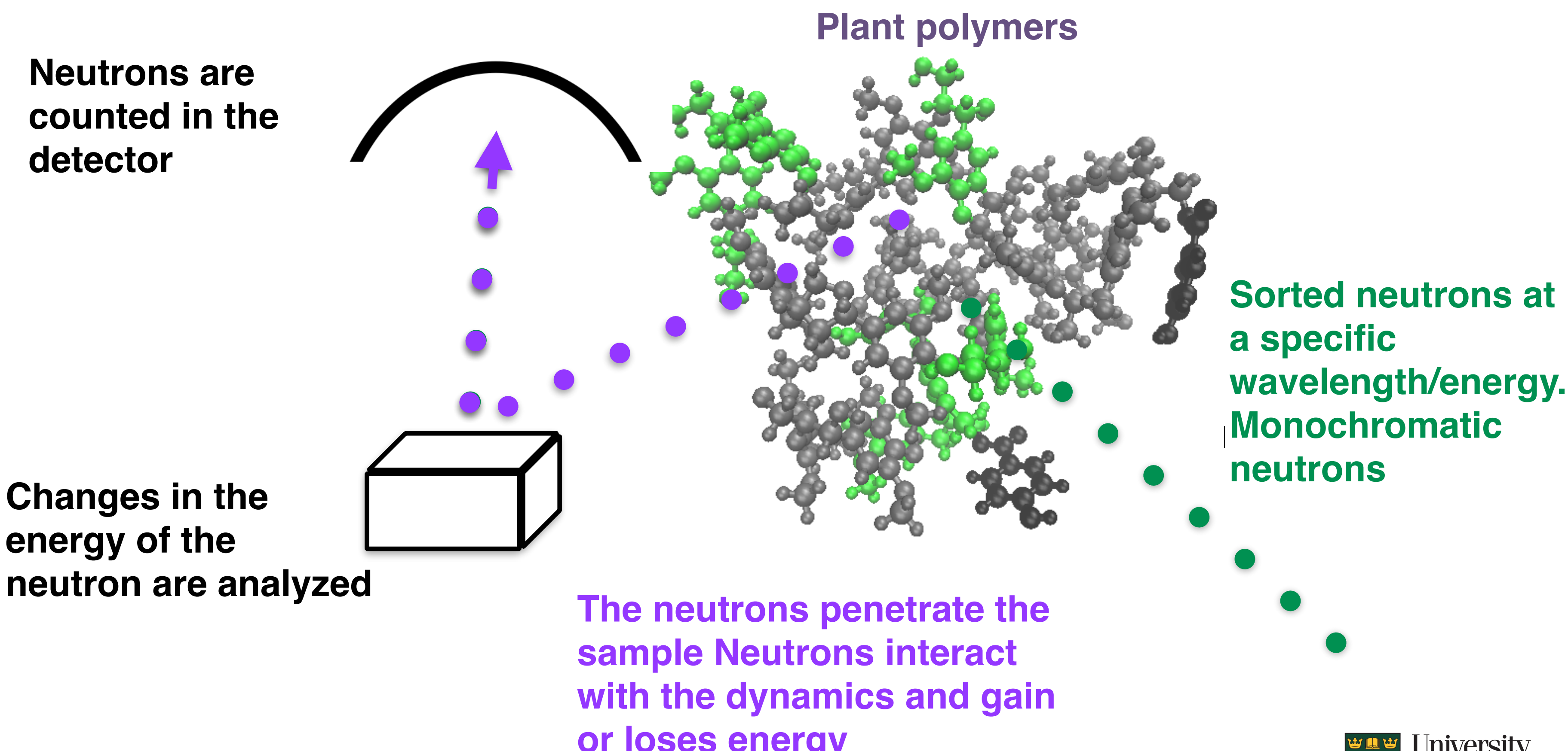
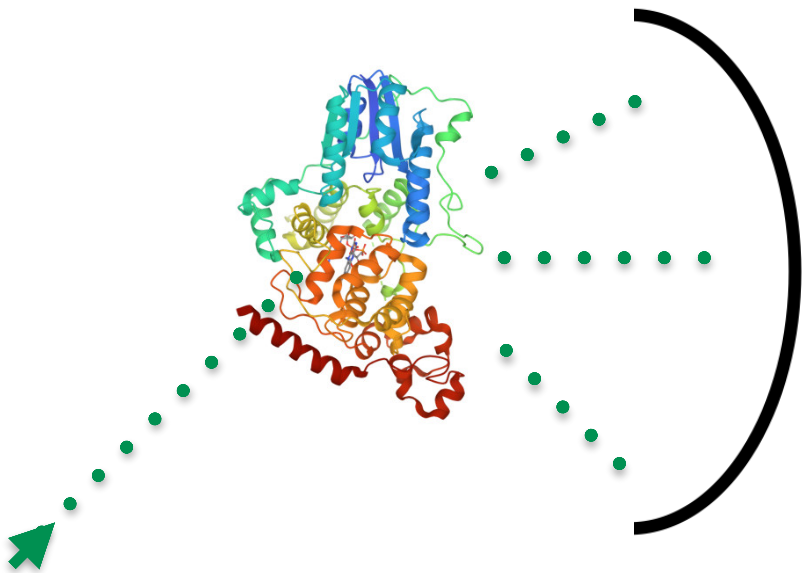
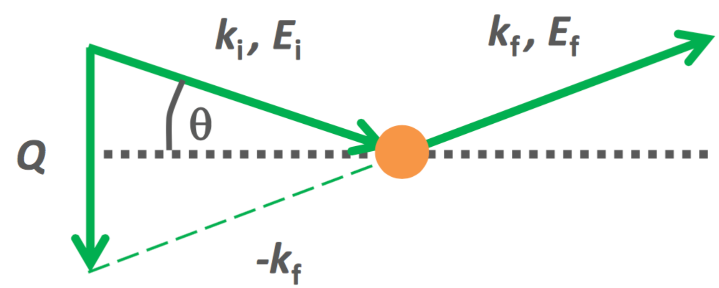


# Neutron Scattering

- Scattering properties of sample depend only on momentum and energy
  - Not on neutron wavelengths



Elastic scattering:




$$|k_i| = |k_f| = \frac{2\pi}{\lambda}$$

**Conservation of momentum: $Q = k_f - k_i$**
**Conservation of energy: $E = ( h^2 m / 8 \pi^2 ) (k_f^2 - k_i^2)$**

# Neutron Scattering

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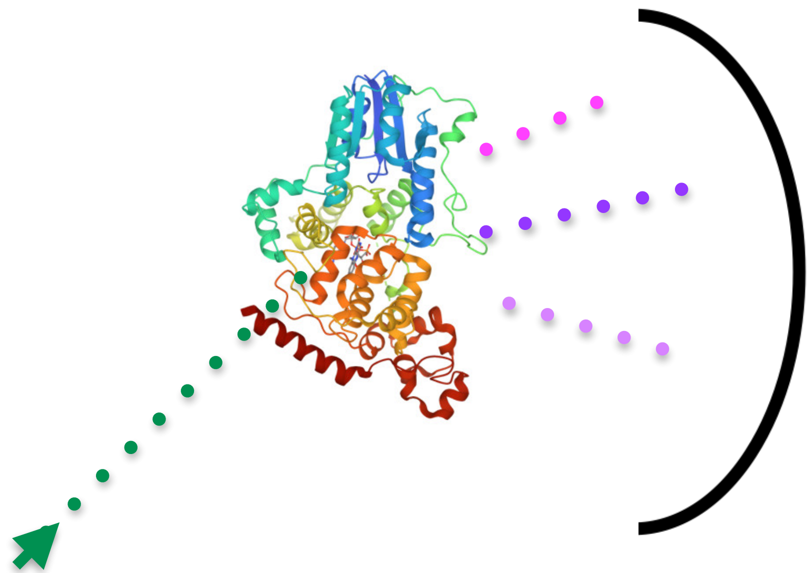
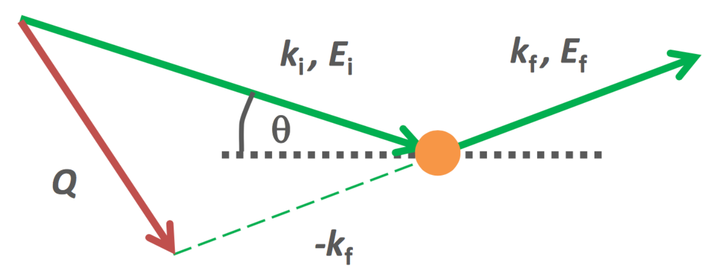


Inelastic scattering:




$$|\boldsymbol{k}_i| \neq |\boldsymbol{k}_f|$$

**Conservation of momentum: $Q = k_f - k_i$**

**Conservation of energy: $E = ( h^2 m/ 8 \pi^2 ) (k_f^2 - k_i^2)$**

# Neutron Scattering

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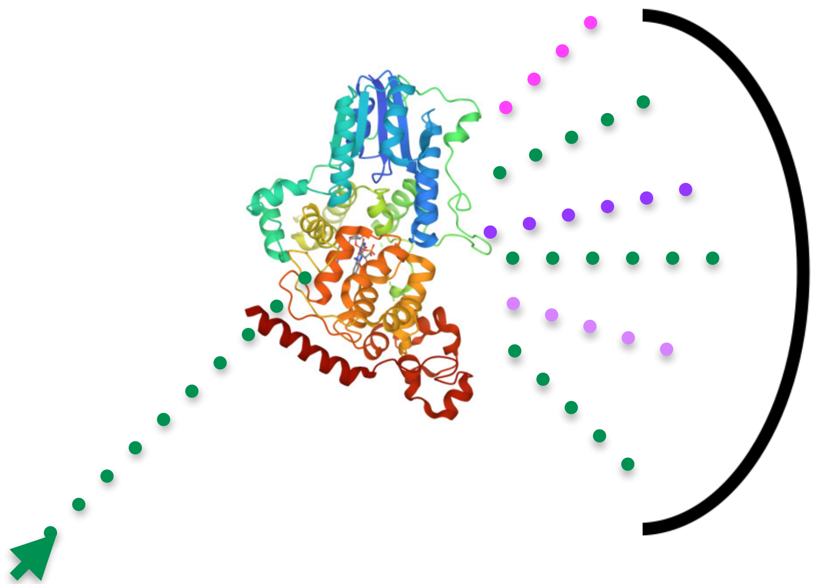


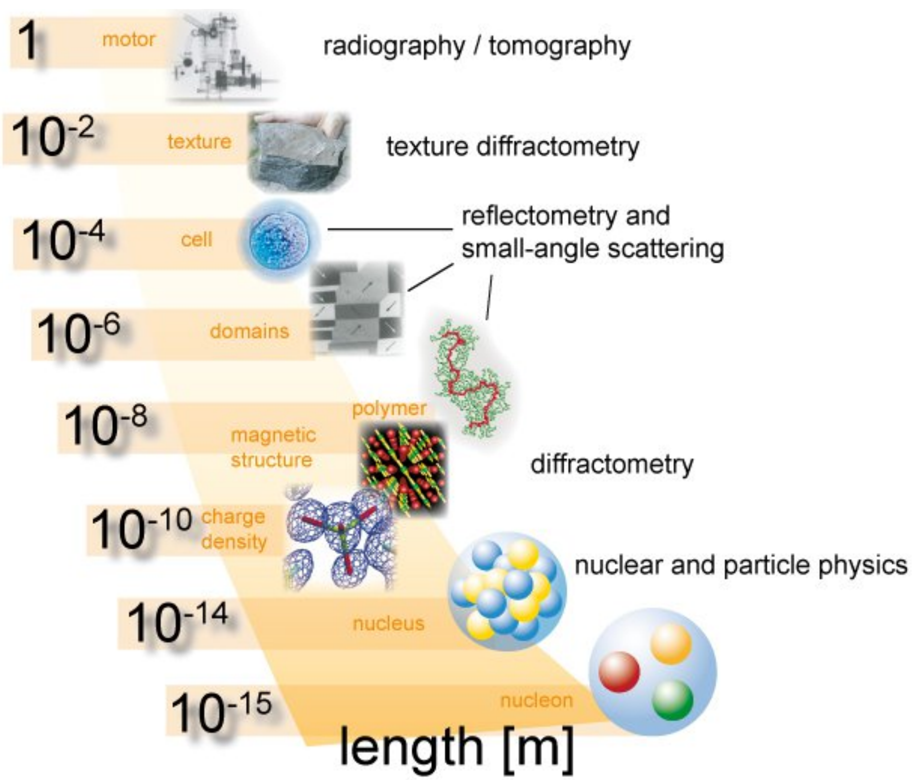
- Many types of neutron scattering instrument are required because the accessible Q and E depend on neutron energy
- Resolution and detector coverage have to be tailored to the science for such a signal-limited technique

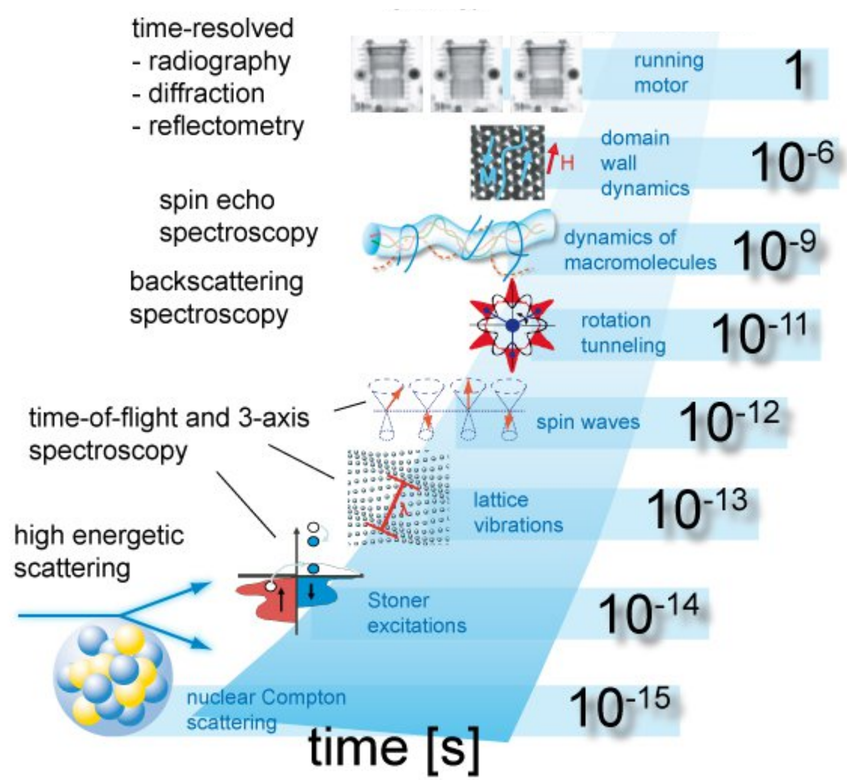
Conservation of momentum: $Q = k_f - k_i$

Conservation of energy: $E = ( h^2 m / 8 \pi^2 ) (k_f^2 - k_i^2)$

# Neutron Scattering

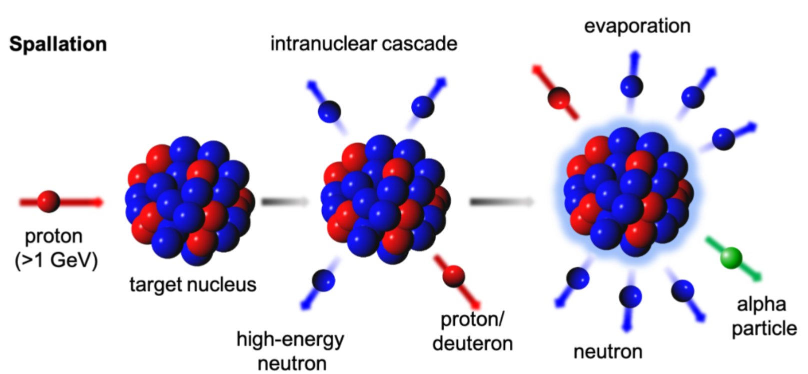
- **Neutrons can be used to investigate different time- and length-scales**

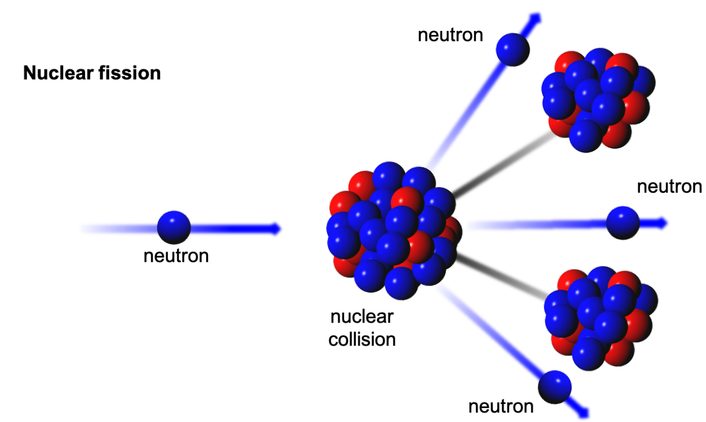


# Neutron Scattering

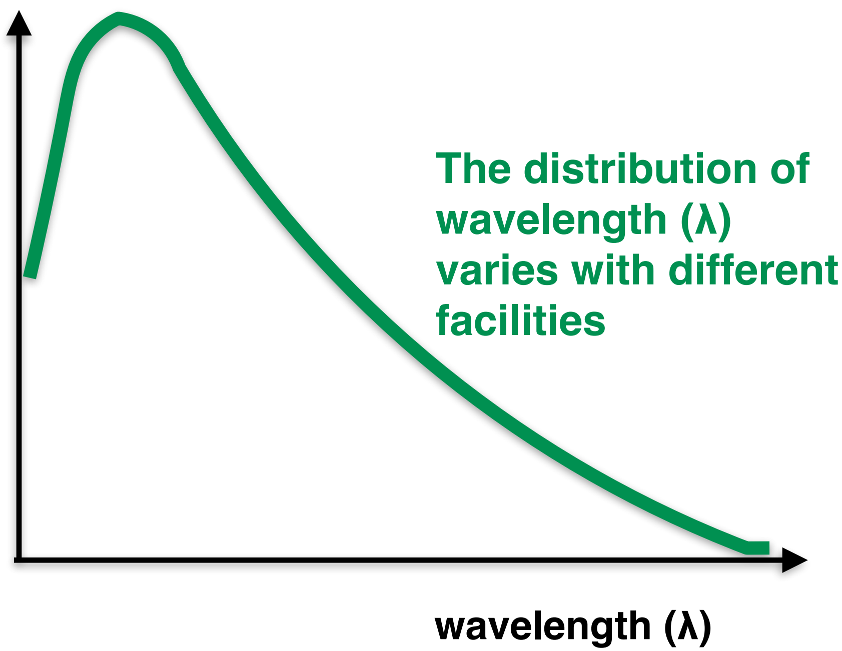
- Neutron Scattering Requires Intense Sources of Neutrons
  - Neutrons for scattering experiments can be produced either by:
    - Nuclear fission in a reactor
    - Spallation when high-energy protons strike a heavy metal target (W, Ta, or U)



# Neutron Scattering

- **Using the beam to investigate different sample properties**



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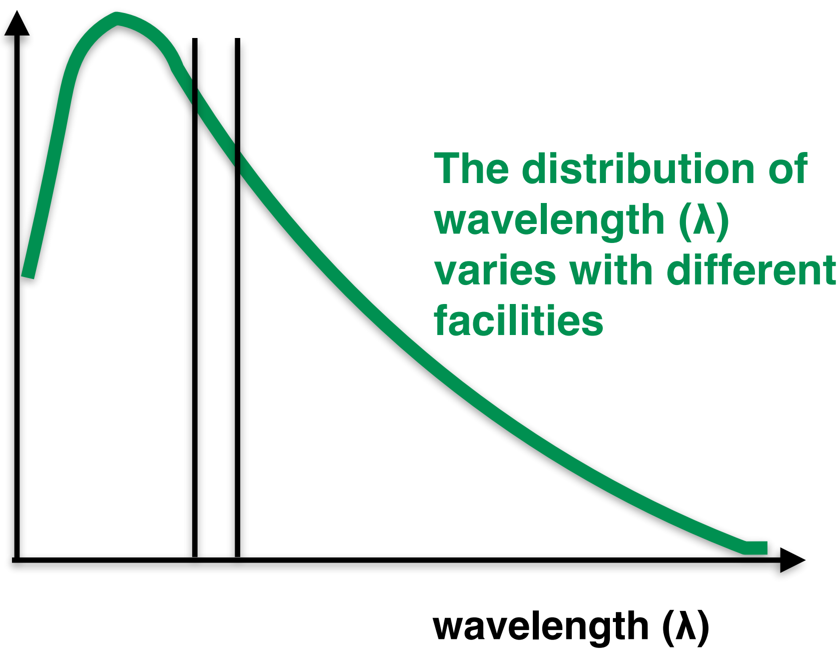
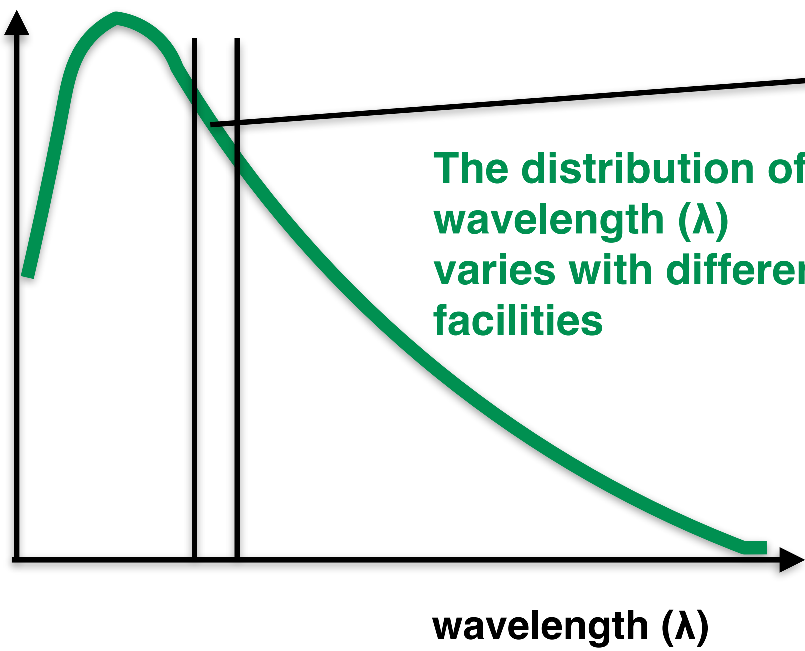



- Each instrument uses a different part of the beam

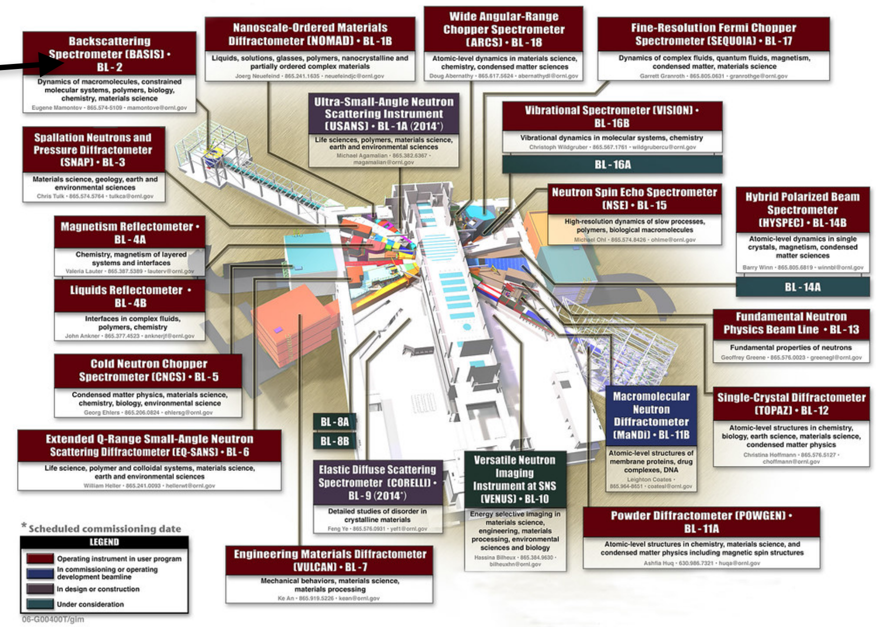
# Neutron Scattering

- **Using the beam to investigate different sample properties**




**The distribution of wavelength (λ) varies with different facilities**

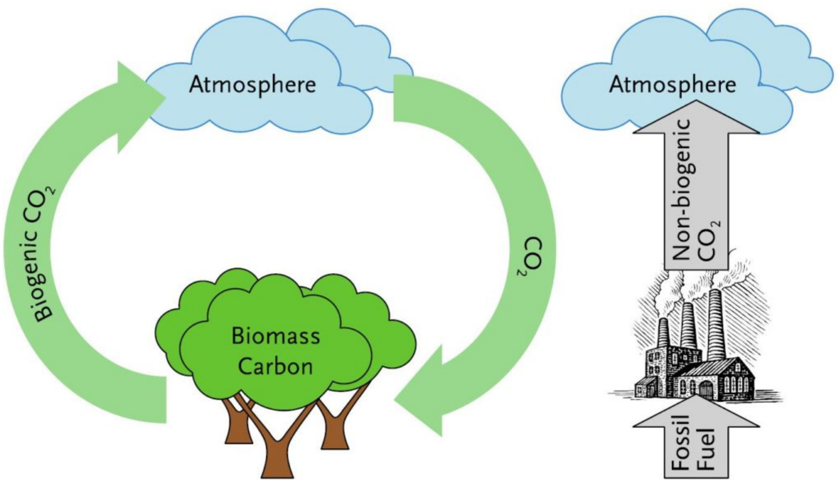
**SNS instrument layout (ORNL)**




- **Each instrument uses a different part of the beam**

# Motivation

- **Sustainability**

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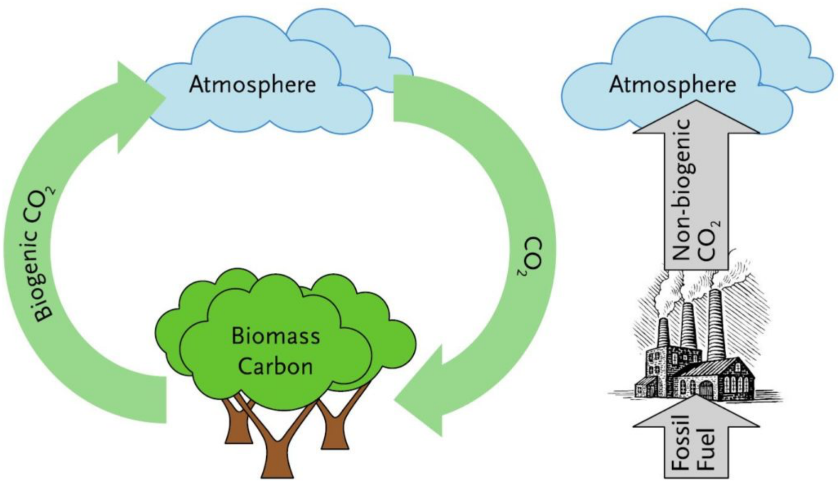


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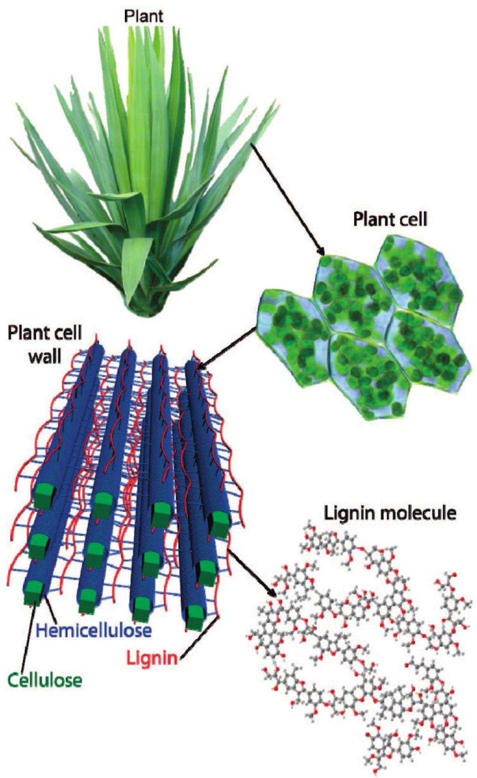
**Lignin is a class of complex organic polymers that form key structural materials in the support tissues of plants**



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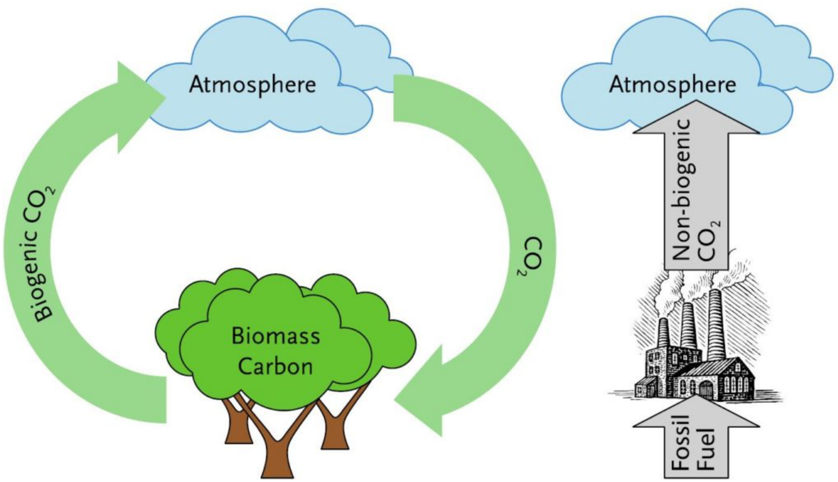


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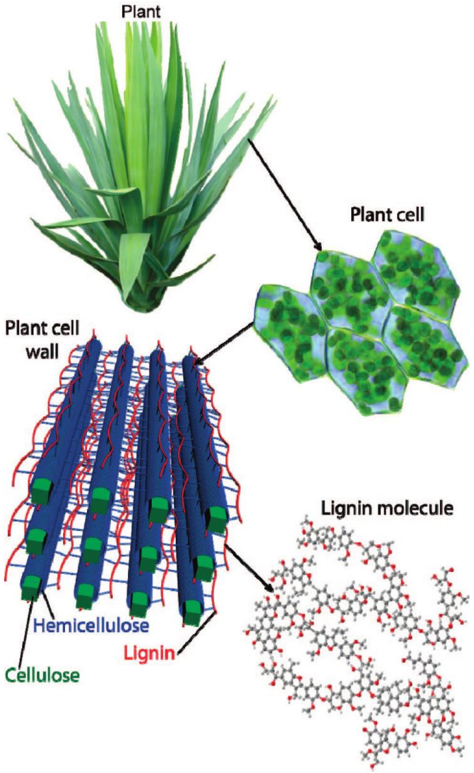
**This study aims to understand the underlying processes that cause the dynamical increase of lignin motion**

**Lignin is a class of complex organic polymers that form key structural materials in the support tissues of plants.**



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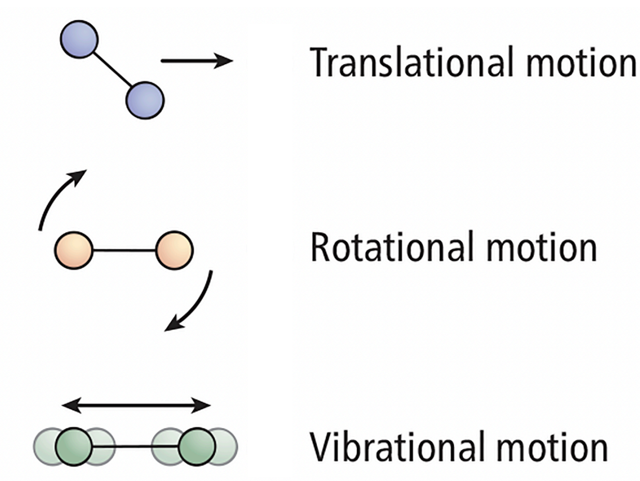
# Neutron Scattering: Biomass

- To facilitate deconstruction it is necessary to "soften" lignin
- Increasing lignin atomic fluctuations



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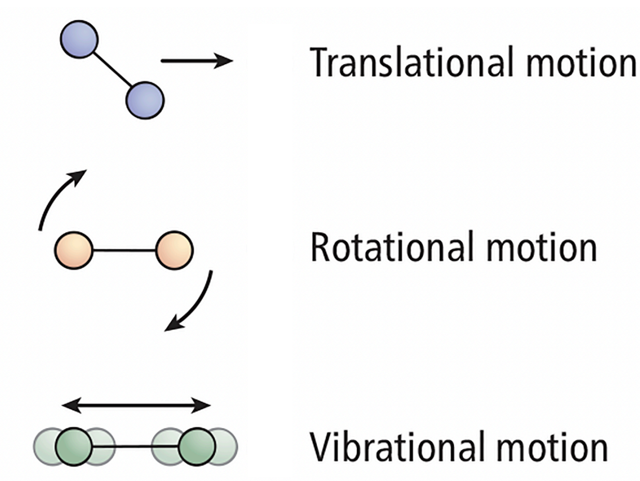


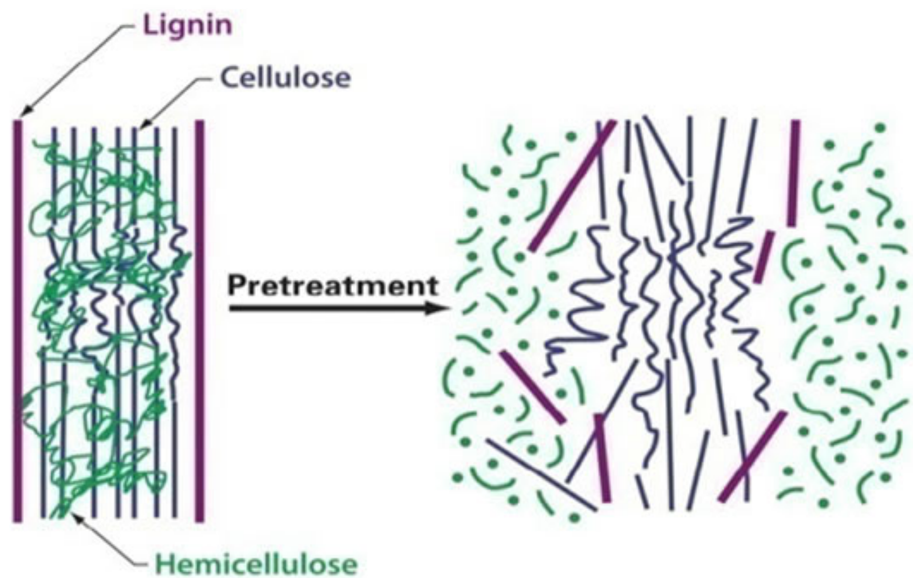


- **Pretreatment involves high temperatures and solvents**

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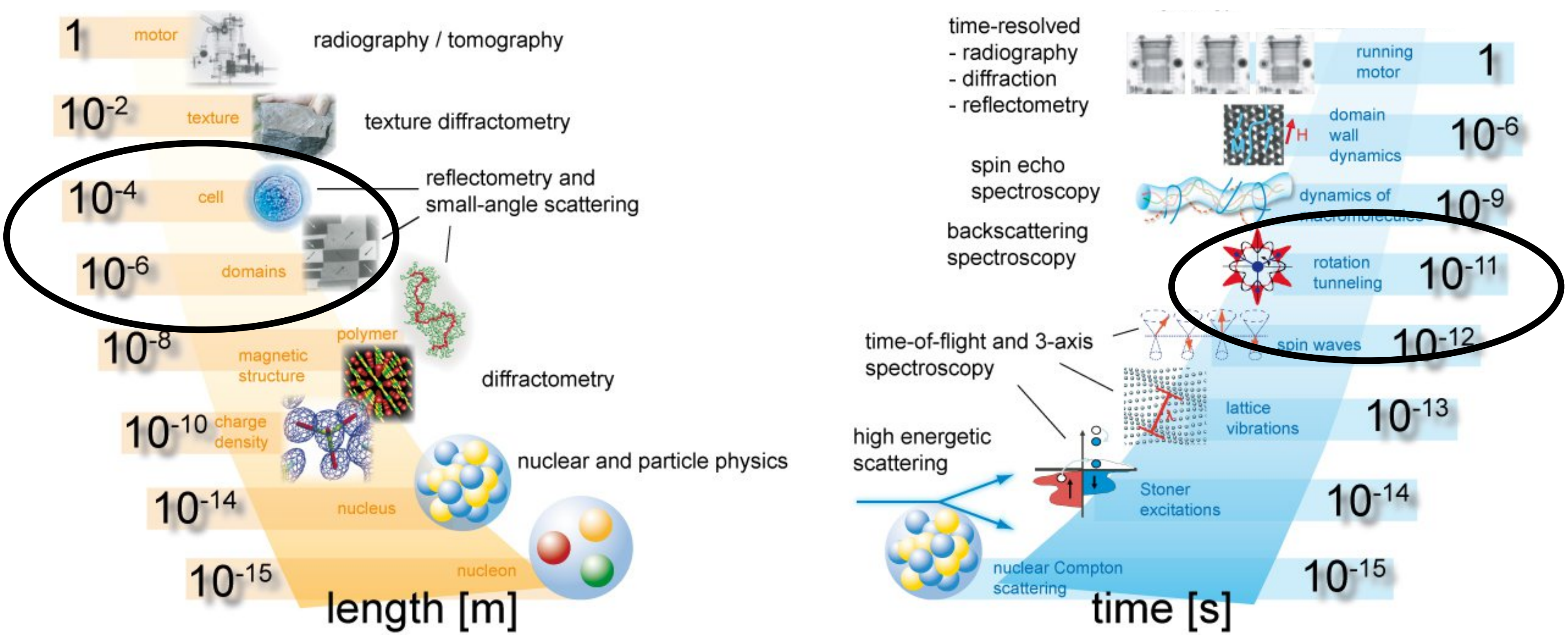




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# Neutron Scattering: Biomass

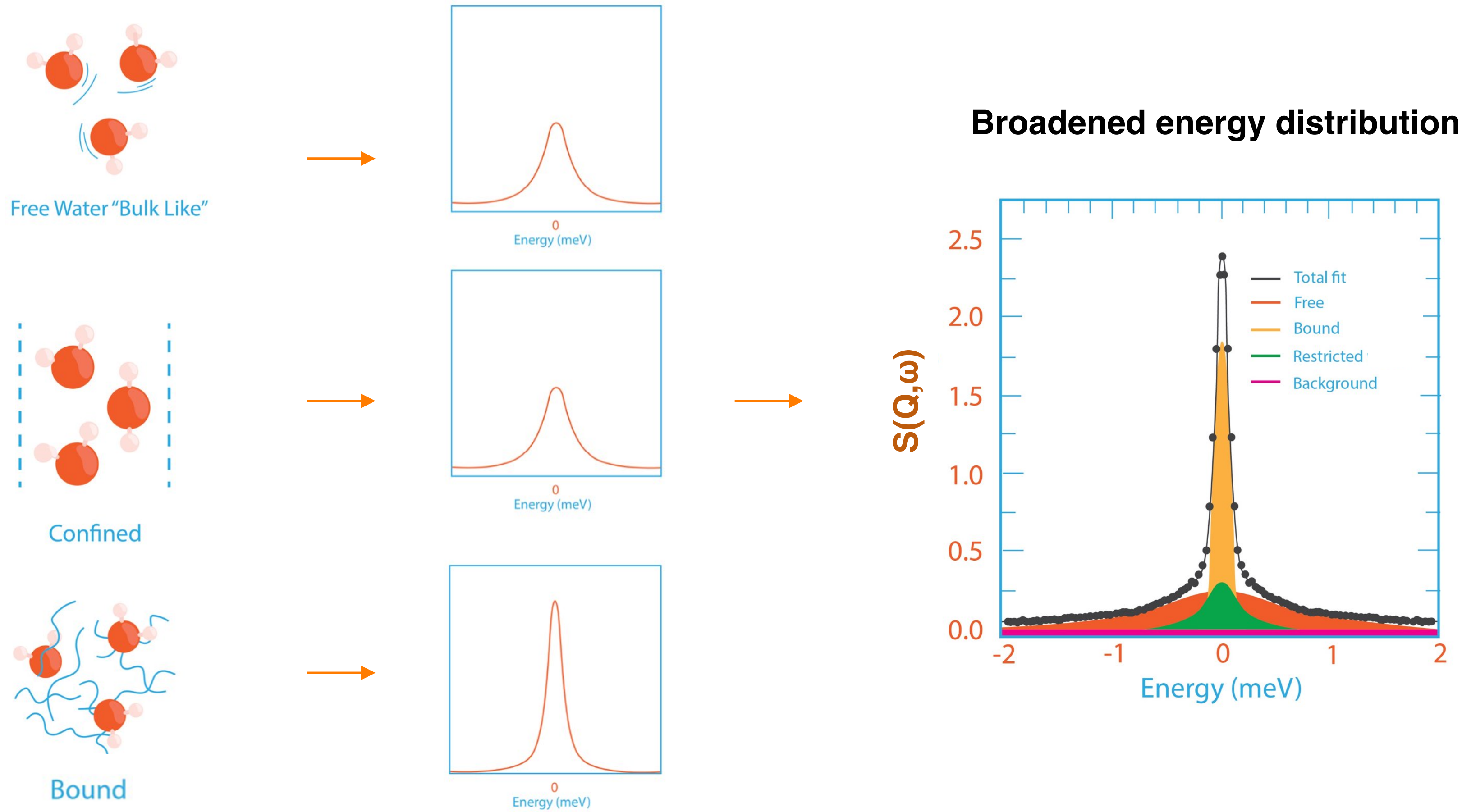
- **$S(Q,\omega)=S_{inc}(Q,\omega)+ S_{coh}(Q,\omega)$ -total signal is weighted by its respective cross-section of each coherent and incoherent term**

| | $^{1}H$ | $^{2}D$ | C | O | Al | Si | Sr |
|---|---|---|---|---|---|---|---|
| $\sigma_{coh}$ | 1.76 | 5.59 | 5.55 | 4.23 | 1.49 | 2.12 | 6.42 |
| $\sigma_{inc}$ | 80.27 | 2.05 | <0.01 | <0.01 | <0.01 | 0 | 0 |

(Dianoux, A. J. and Lander, G. (Eds.) Neutron data booklet. ISBN: 0-9704143-7-4).

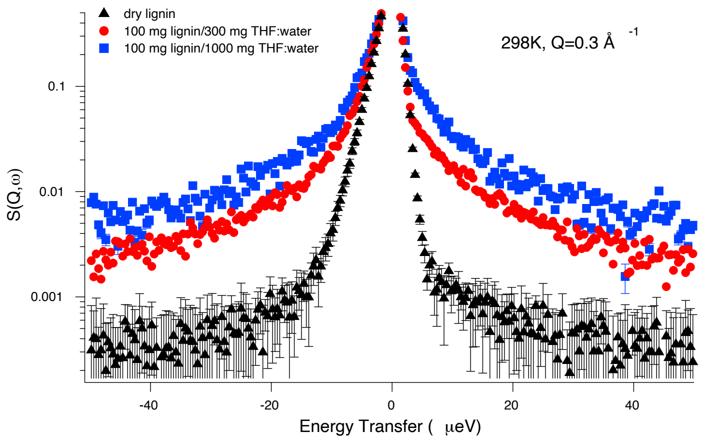
# Neutron Scattering: Biomass

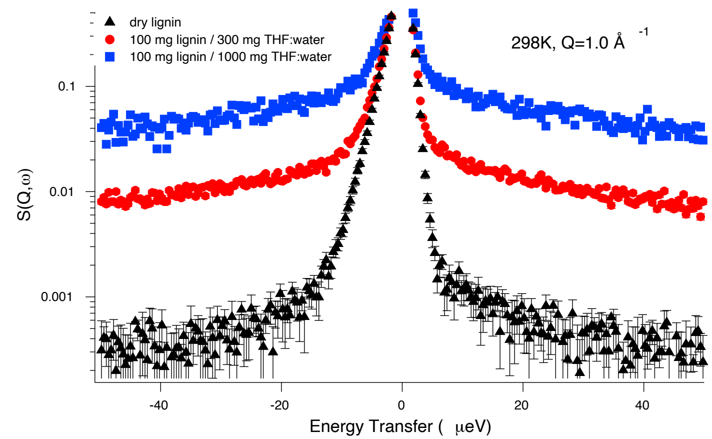
- **Quasi-elastic neutron scattering**

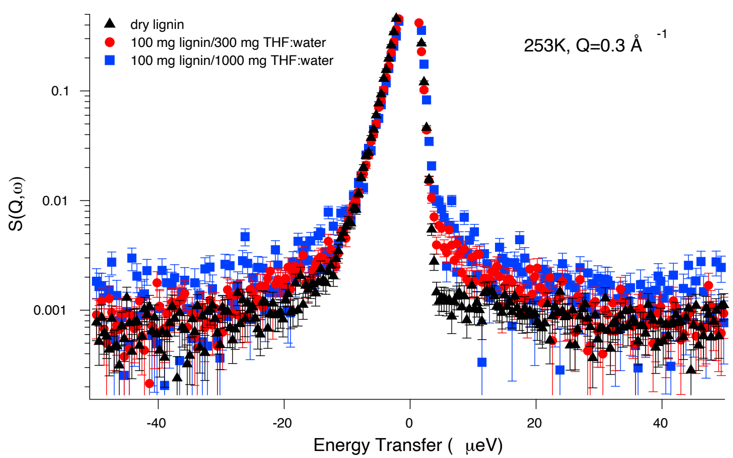


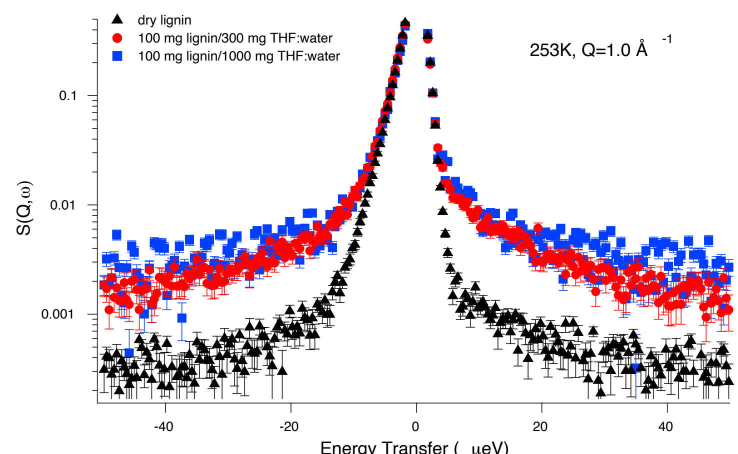
# Neutron Scattering: Biomass

- **Experimental data collected at SNS at Oak Ridge National Laboratory**
- **Dynamics "activities" at different temperatures**



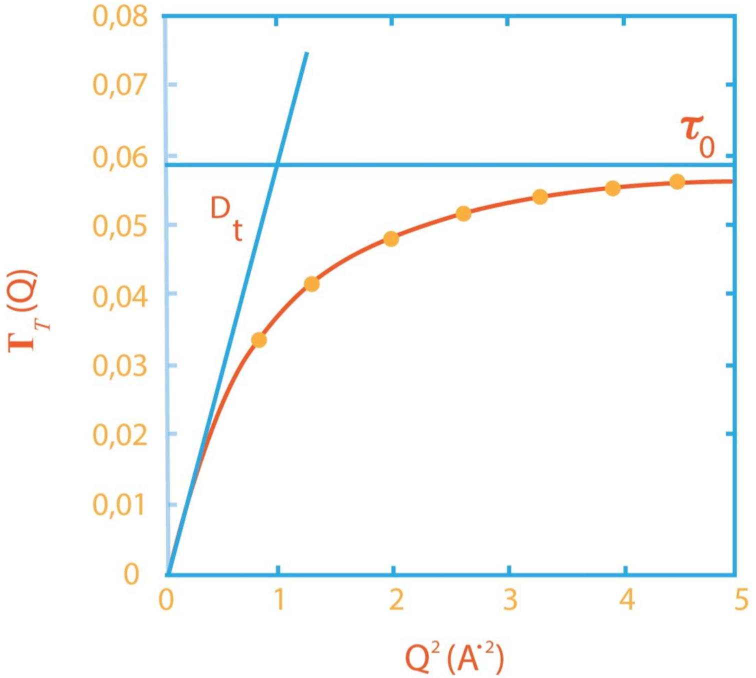



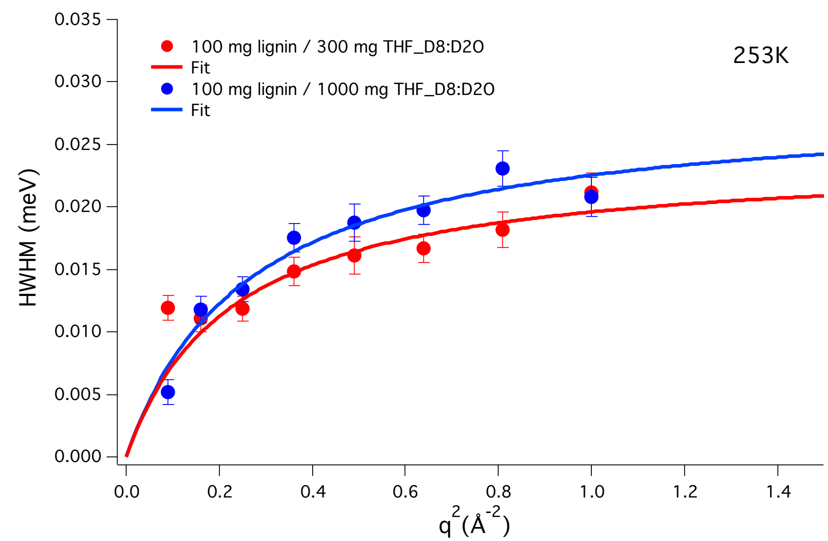



# Neutron Scattering: Biomass

- **The broadening as a function of wavevector describes the dynamics**

$$\Gamma_T(Q) = \frac{D_t Q^2}{1 + D_t Q^2 \tau_0} \quad \text{and} \quad D_t = \frac{L^2}{6\tau_0}$$



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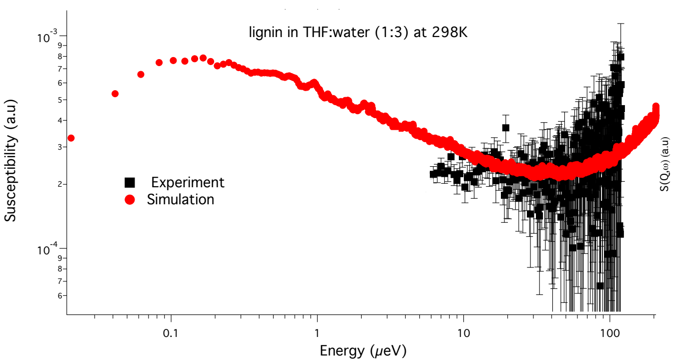
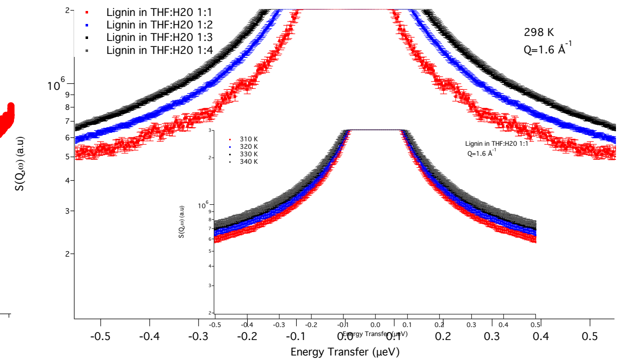
# Conclusion

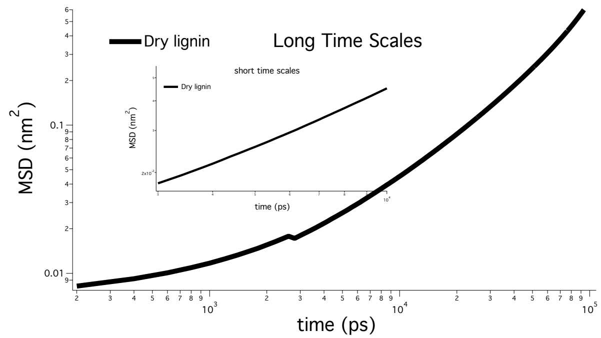
## validating models



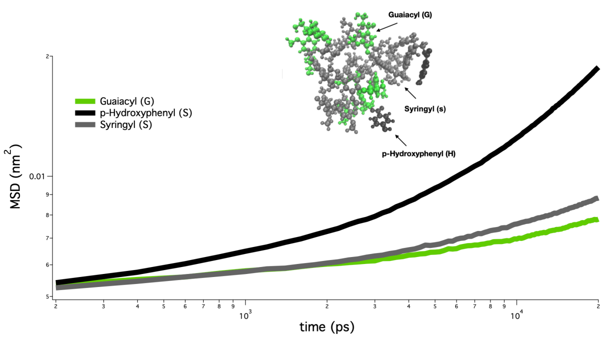

## temperature and solvent



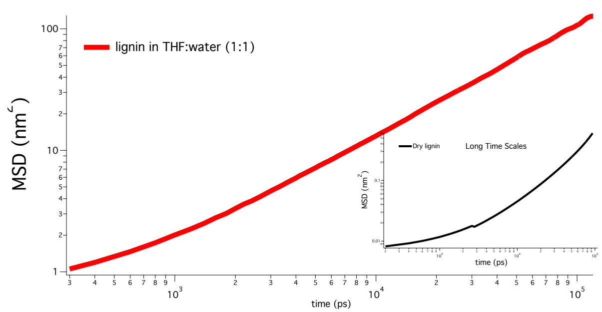

## timescales



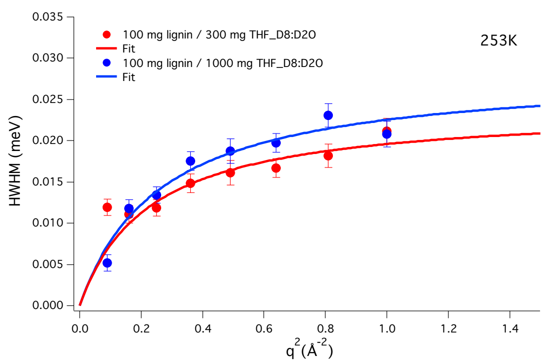

## choosing the right plant




## solvent and dynamics




## dynamics at low temperatures

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# Acknowledgement


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SYLVIA FEDORUK CANADIAN CENTRE FOR NUCLEAR INNOVATION

# Thank you

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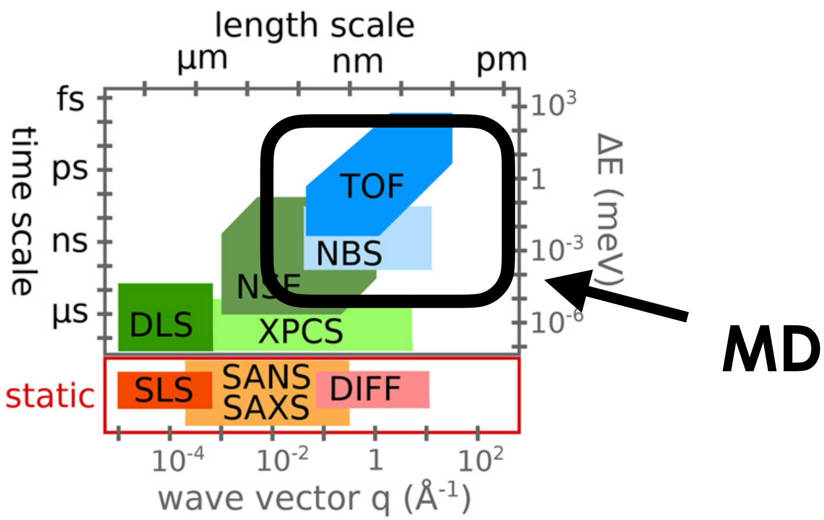
# Methods: Molecular dynamics simulations (MD) and QENS




| | |
|---|---|
| DIFF | diffraction |
| DLS | dynamic light scattering |
| NBS | neutron backscattering |
| NSE | neutron spin-echo |
| SANS | small angle neutron scattering |
| SAXS | small angle X-ray scattering |
| SLS | static light scattering |
| TOF | neutron time-of-flight |
| XPCS | X-ray photon correlation spectroscopy |

- MD probes similar length- and time-scales as QENS.
- MD access a broad range of time scales and provides a full atomistic model of the system.

# Sample and Model

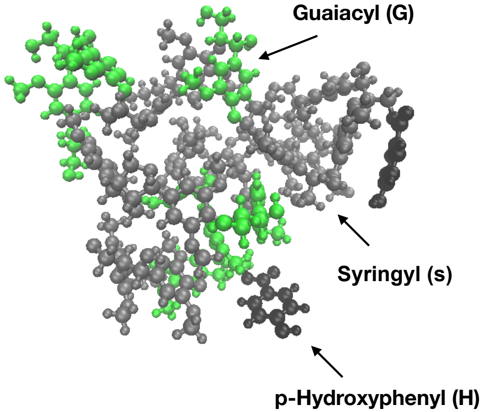
**Building a computational model with the same "properties" as the sample**

**Extracted native lignin**

→ **Density**

**Composition** →

**Computational model of native lignin**



# Dynamics in lignin: MD