# *Dynamics*
## and
# Neutron Scattering

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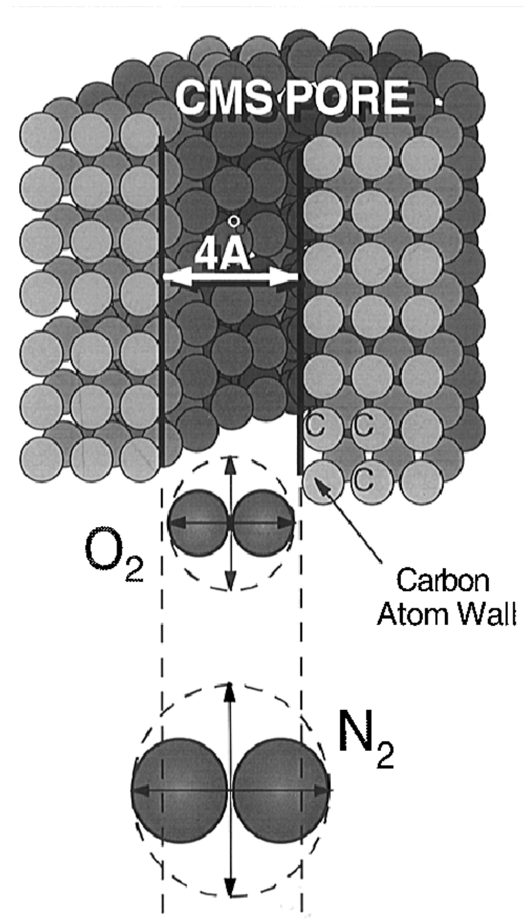
# *Dynamics*

## Chemical Separation

Molecular sieves separate chemical species via different rates of diffusion

Carbogenic molecular sieves are used to separate oxygen and nitrogen. The ratio of diffusivities is ~ 20:1.

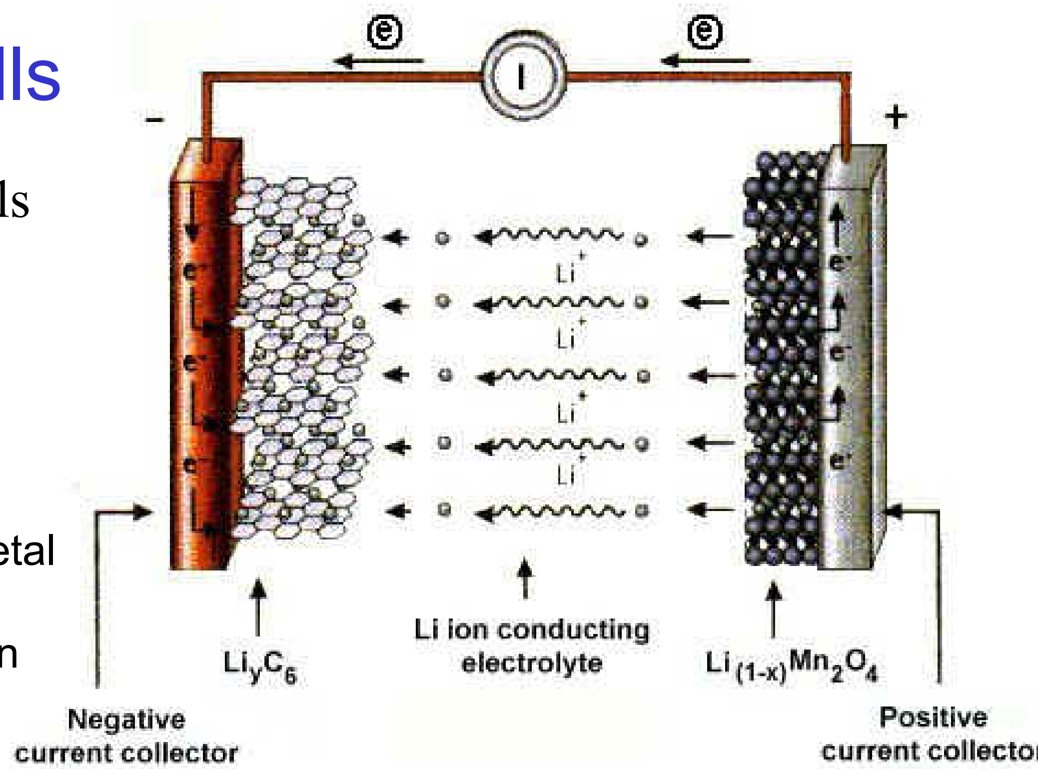


# *Dynamics*

## Batteries and Fuel Cells

Solid state batteries and fuel cells depend on the rapid diffusion of ions both in the electrodes and through the electrolyte.

Li ions move from a transition metal oxide to a carbon electrode by traversing a polymer electrolyte in response to a flow of electrons supplied by an external circuit.

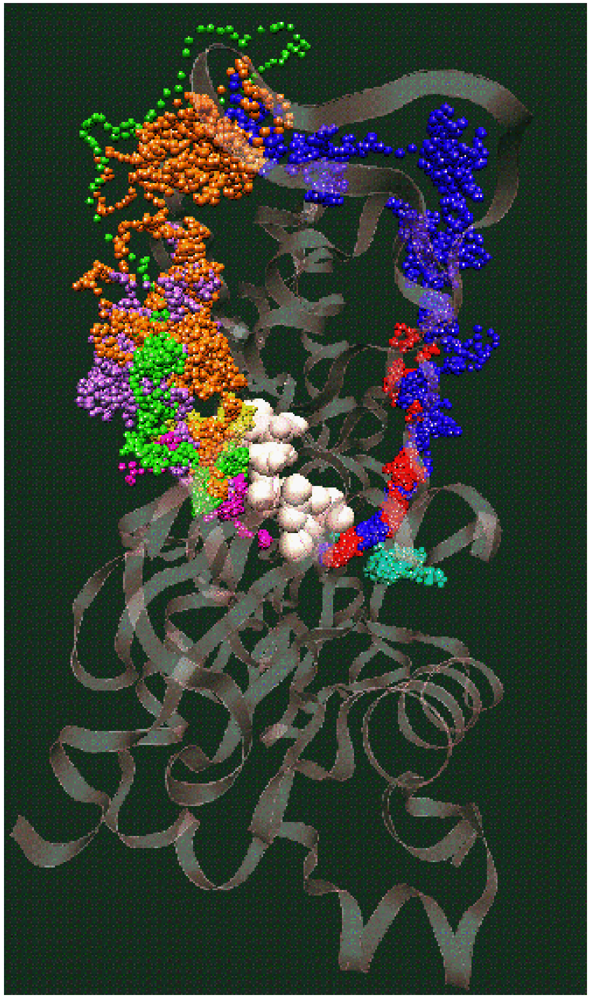


# Dynamics

## Protein Function

The biological activity of a protein depends on its ability to fold into its own native state. Protein function relies on structure and dynamics.

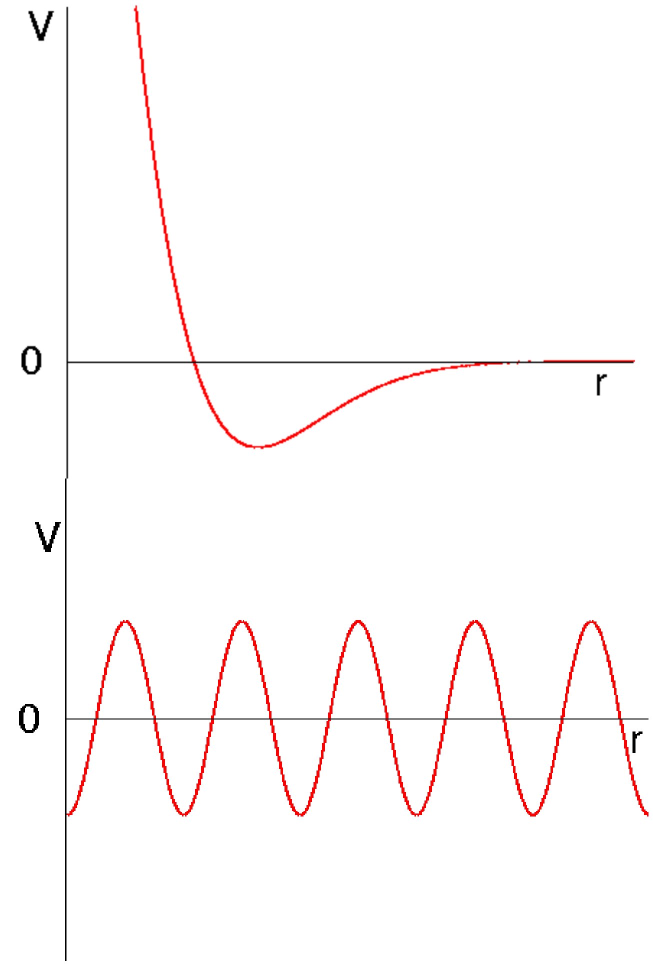
Dynamic actin based structures are important in cell shape changes and motility, cytokinesis and other processes. Here we see the diffusion pathways for water to reach the active site. These are believed to be relevant for the dissociation of phosphate after hydrolysis.



# Dynamics

## Fundamental Information on Interactions in Materials

Structural probes yield indirect information on interactions in materials by locating the minimum of the potential.  Dynamical probes, including neutron scattering, reveal information on the shape of the potential.



# Why Neutrons

## Nuclear Interaction

- strong but very short ranged
- no electrostatic interaction (overall interaction is weak)
  => neutrons easily penetrate experimental apparatus
- scattering power varies “randomly” from isotope to isotope
  => isotopic labeling
  => scattering from light elements comparable to that from heavy elements
- nuclear spin dependence of the interaction

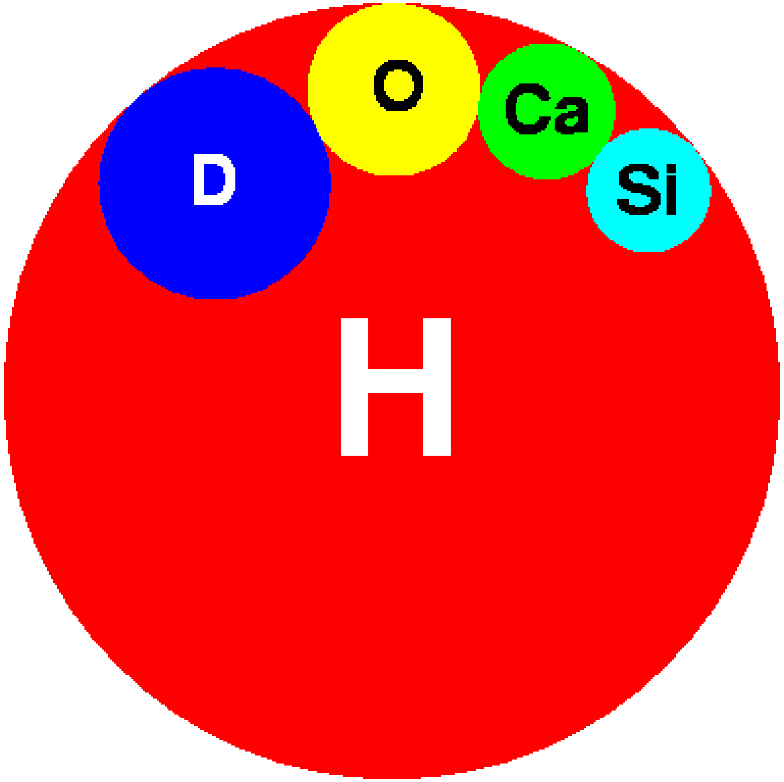
# Nuclear Interaction

scattering power varies "randomly" from isotope to isotope

Cross section ($\sigma$) - Area related to the probability that a neutron will interact with a nucleus in a particular way (*e.g.* scattering or absorption)

For systems containing a reasonable proportion of H atoms, scattering from H tends to dominate

For a single nucleus $\sigma \sim 10^{-24}$ cm$^2$




Relative total scattering cross sections for a few isotopes

# Nuclear Interaction

- scattering power varies “randomly” from isotope to isotope
- nuclear spin dependence of the interaction

Not all nuclei in a sample consisting of only one element or even only *isotope* necessarily scatter identically

**=> RANDOMNESS**

If the scattered neutron waves from the different nuclei have RANDOM relative phases, they don’t interefere

**=> *IN*COHERENT SCATTERING**

If the scattered neutron waves from the different nuclei have definite relative phases, they can interefere

**=> COHERENT SCATTERING**

# Why Neutrons

## Wavelength ~ Å's

- comparable to interatomic and intermolecular distances
- comparable to x-rays

=> interference effects

cold neutrons - long wavelengths - longer length scales

# Why Neutrons

## Energy ~ meV's

- comparable to the time scale of many motions in materials

  => inelastic scattering from vibrations, diffusion, reorientations, and relaxational processes can be observed

- light  E ~ eV's  $\lambda$ ~ 1000 A's  Q ~ 0 (selection rules)
- x-rays  E ~ keV's  $\lambda$ ~ A's

cold neutrons - lower energies - longer time scales

1 meV ◆ 8 $cm^{-1}$ ◆ 240 GHz ◆ 12 K ◆ 0.1 kJ/mol ~ ps

# Why Neutrons

Wavelength ~ Å's ⇔ Energy ~ meV's

=> geometry of the motion!

# Scattering Geometry

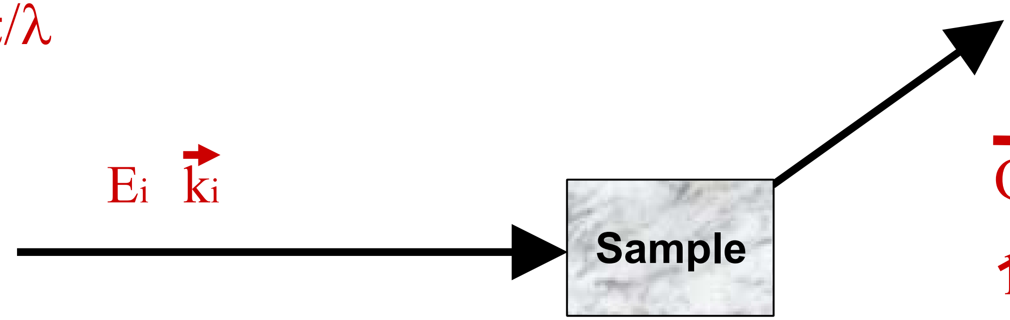
momentum = $\hbar\vec{k}$

$k = 2\pi/\lambda$

energy = $(\hbar k)^2/(2m)$

$E_f$ $\vec{k}_f$

$E_i$ $\vec{k}_i$




$\vec{Q} = \vec{k}_i - \vec{k}_f$

$\hbar\omega = E_i - E_f$

Measure the number of scattered neutrons
as a function of Q and $\omega$

=> $S(Q,\omega)$ (the scattering function)

depends ONLY on the sample

# Scattering function

$$S(Q,\omega) = S_{inc}(Q,\omega) + S_{coh}(Q,\omega)$$

$S_{inc}(Q,\omega)$ is the time and space Fourier transform of the *SELF* correlation function

$S_{coh}(Q,\omega)$ is the time and space Fourier transform of the *PAIR* correlation function

* Spin Echo measures the INTERMEDIATE scattering function $I(Q,t)$

# Why Neutrons

## Magnetic Moment

- neutrons interact directly with magnetic materials

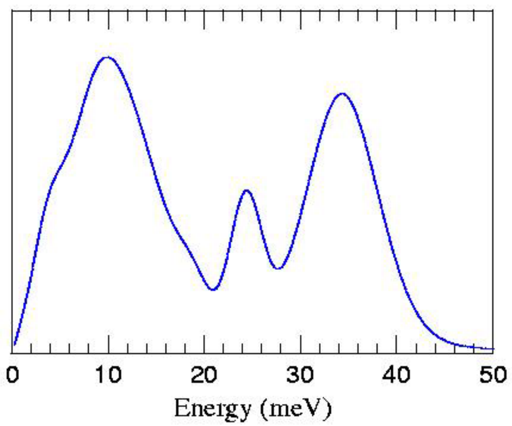
  => *magnetic structures*

  => *magnetic excitations*

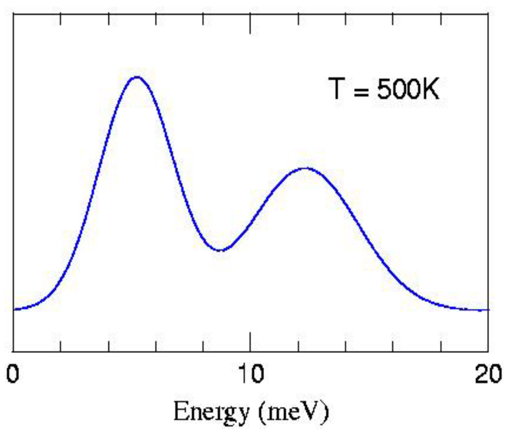
# Things you can do

## Dynamics of Solids

*Glasses* a-$GeSe_2$



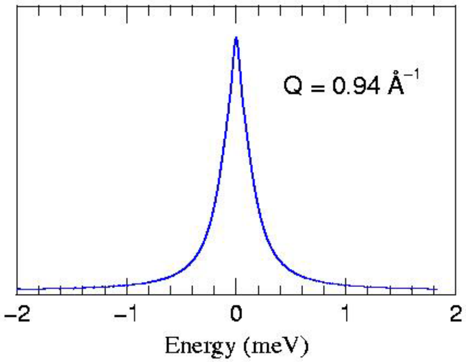

*Phonons in Crystals* $Pb(Zn_{0.33}Nb_{0.67})O_3$



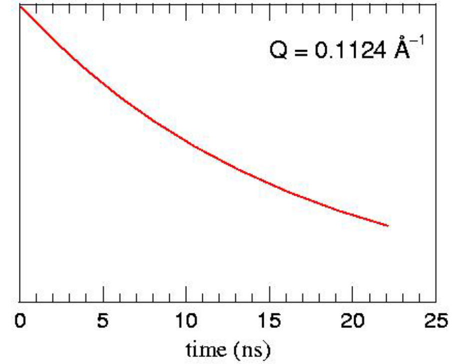
# More things you can do

## Dynamics of Liquids

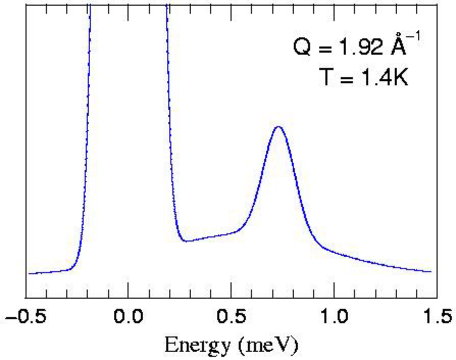
*"Simple" Liquids* Water




*Complex Fluids* SDS solution



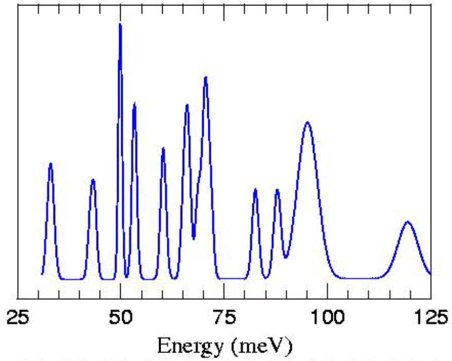

*Quantum Fluids* He in porous glass



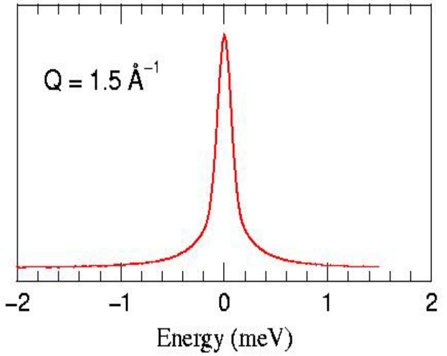
# More things you can do!

## Molecular Systems

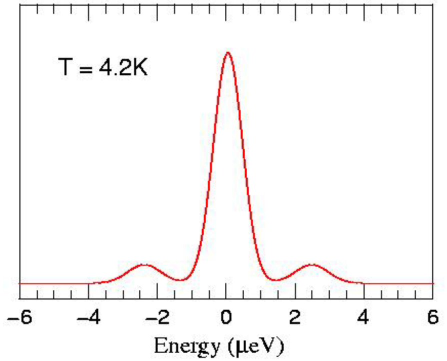
*Vibrational Spectroscopy* $C_{60}$




*Reorientational Dynamics* pyrazine



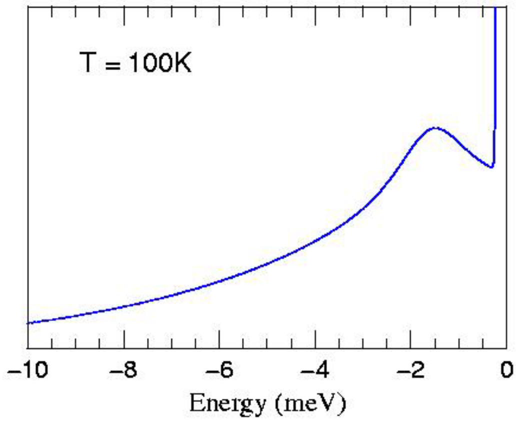

*Rotational Tunneling* $CH_3I$



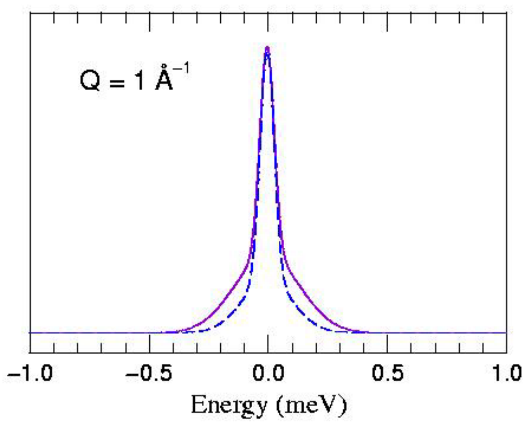
# More things you can do!

## Macromolecules

*Polymers* polycarbonate




*Protein Dynamics* α-lactalbumin



# Even more things you can do!

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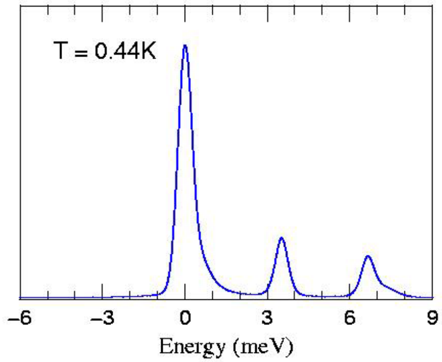
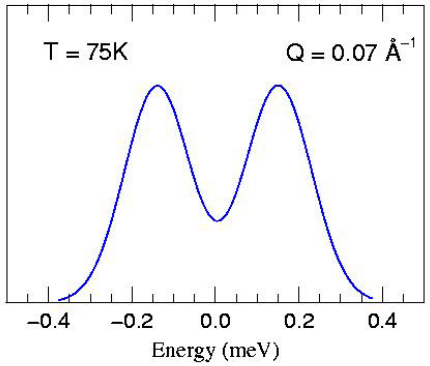
## Magnetic Excitations

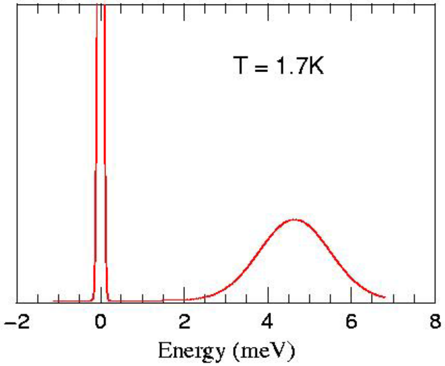
*Crystal Field Splittings* $HoPd_2Sn$



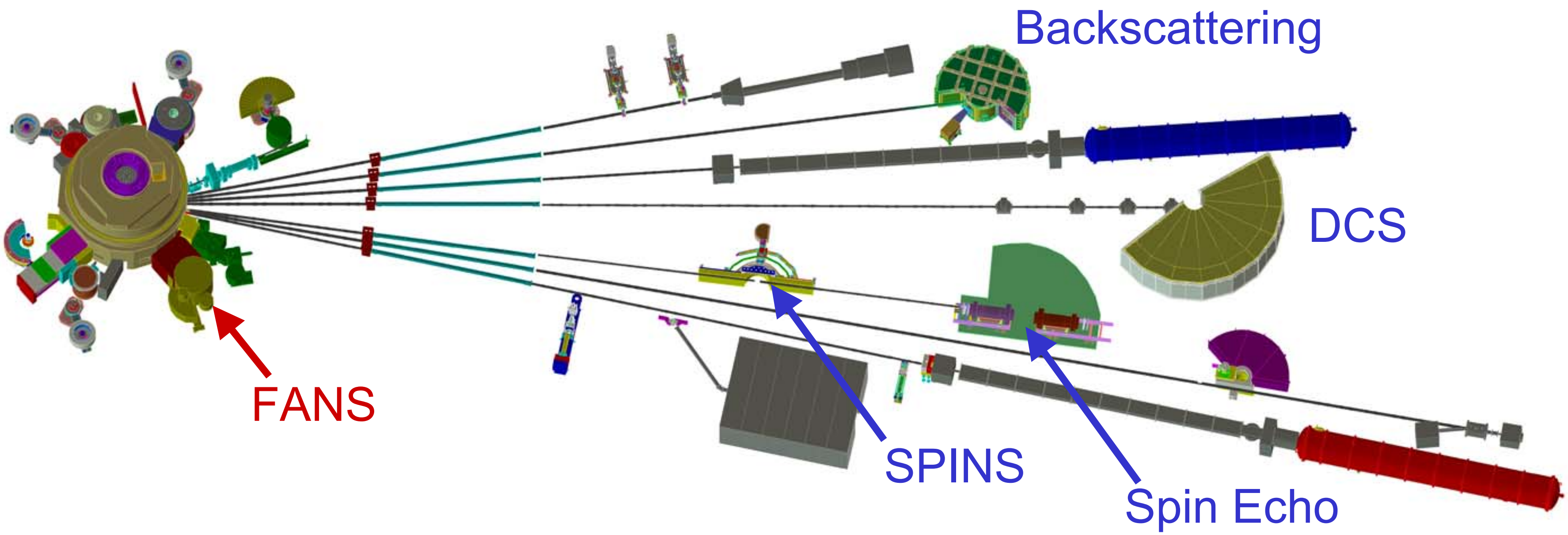

*Spin Waves* $La_{0.85}Ca_{0.15}MnO_3$

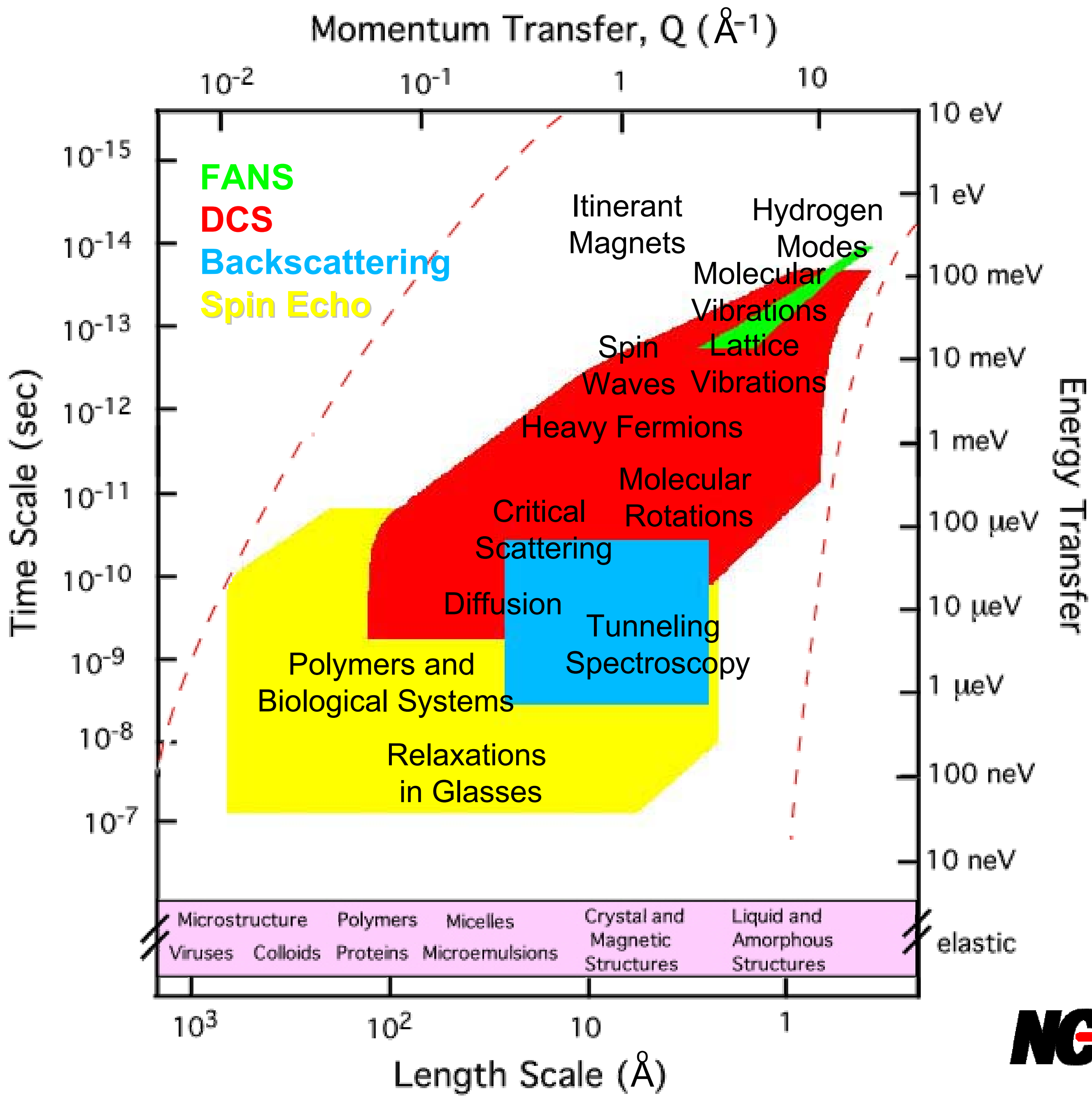



*Local Spin Resonances* $ZnCr_2O_4$



# The NIST Center for Neutron Research





Momentum Transfer, Q (Å-1)
10-2
10-1
1
10
10-15
10-14
10-13
10-12
10-11
10-10
10-9
10-8
10-7
Time Scale (sec)
10 eV
1 eV
100 meV
10 meV
1 meV
100 μeV
10 μeV
1 μeV
100 neV
10 neV
elastic
Energy Transfer
FANS
DCS
Backscattering
Spin Echo
Itinerant Magnets
Hydrogen Modes
Molecular Vibrations
Spin Waves
Lattice Vibrations
Heavy Fermions
Molecular Rotations
Critical Scattering
Diffusion
Tunneling Spectroscopy
Polymers and Biological Systems
Relaxations in Glasses
Microstructure
Polymers
Micelles
Crystal and Magnetic Structures
Liquid and Amorphous Structures
Viruses
Colloids
Proteins
Microemulsions
10³
10²
10
1
Length Scale (Å)

# *Dynamics*
and
# Neutron Scattering

NCNR

The *dynamics* of a system reflect the interatomic and intermolecular interactions which are responsible for the properties of materials

Neutron Scattering is an excellent way to study *dynamics*