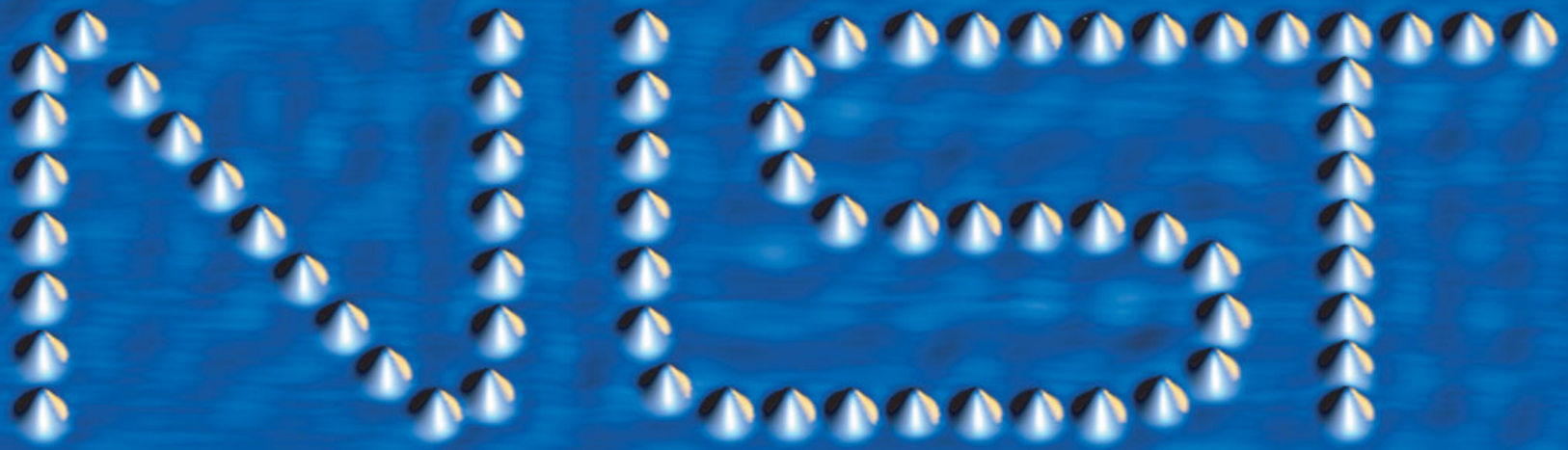
NEUTRON SCIENCE at the NCNR

NIST Center for Neutron Research

March 25, 2014

Rob Dimeo, Director



J. Stroscio/R. Celotta

Promoting U.S. innovation and industrial competitiveness by advancing

measurement science, standards, and technology

in ways that enhance economic security and improve our quality of life.

NIST LABORATORIES

Physical Measurements Laboratory

Material Measurements Laboratory

Engineering Laboratory

Information Technology Laboratory

Communication Technology Laboratory

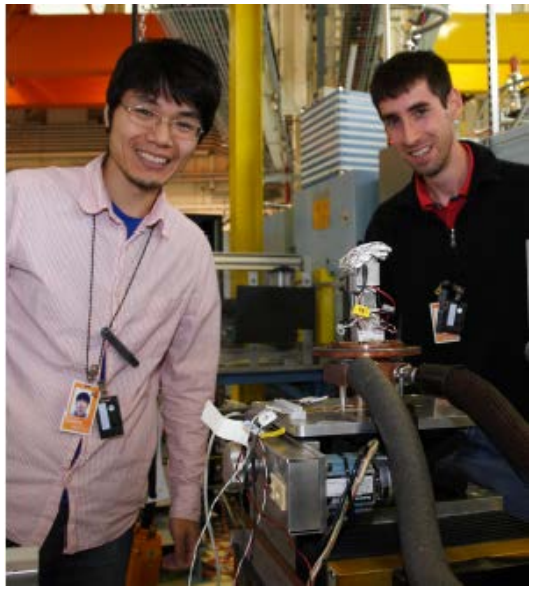
Center for Nanoscale Science and Technology

NCNR

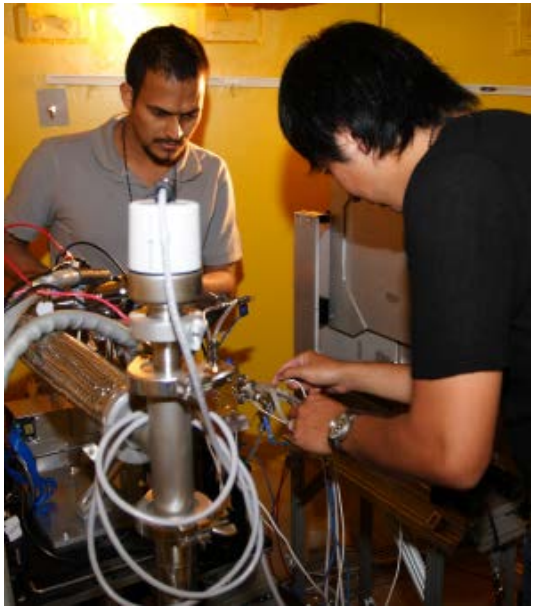
MEASUREMENT LABORATORIES

TECHNOLOGY LABORATORIES

USER FACILITIES



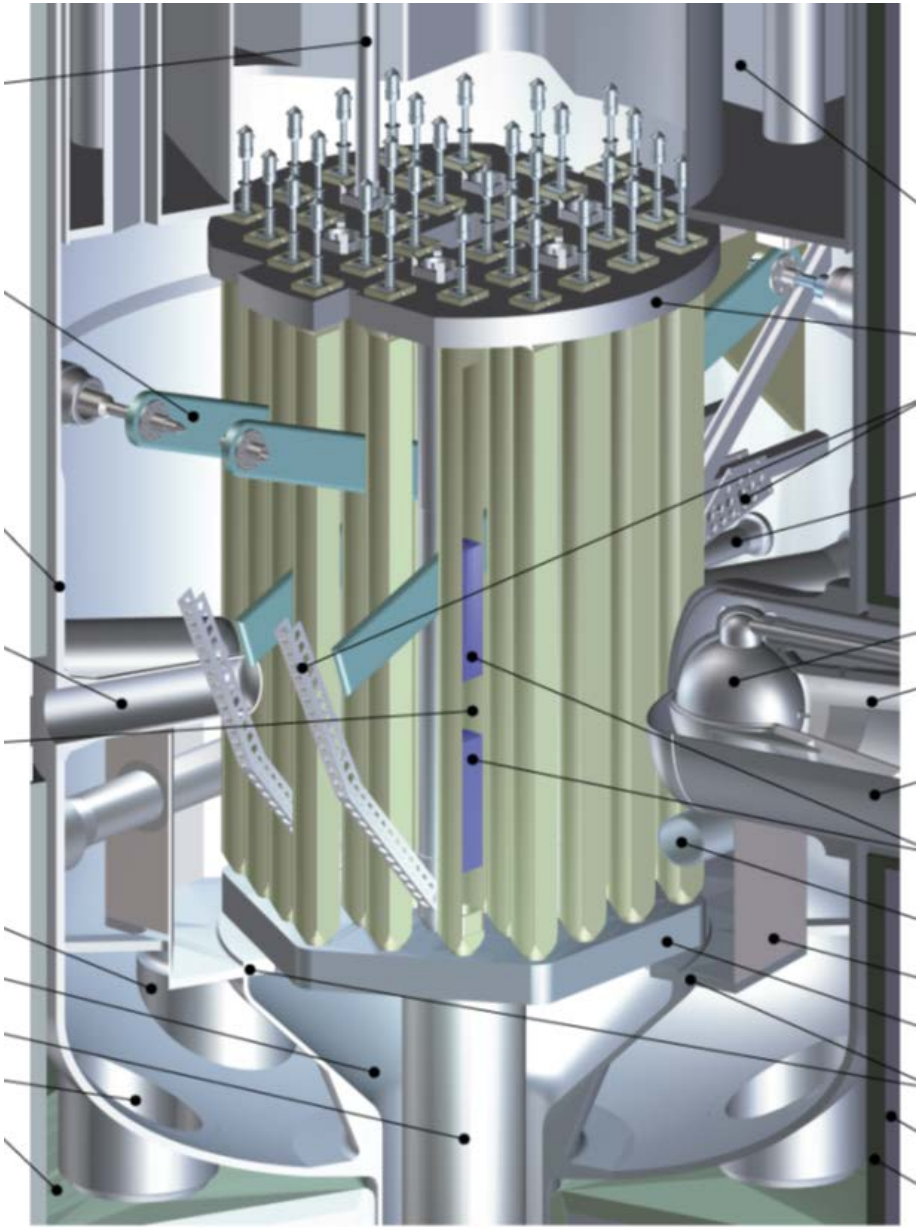
…assure the availability of neutron measurement capabilities to meet the needs of US researchers from industry, university, and government agencies.



June 2013
Photo credit: Brian Renegar

NEUTRON SCATTERING FUNDAMENTALS

NEUTRON PRODUCTION



20 MW
D_2O moderated
30 fuel elements

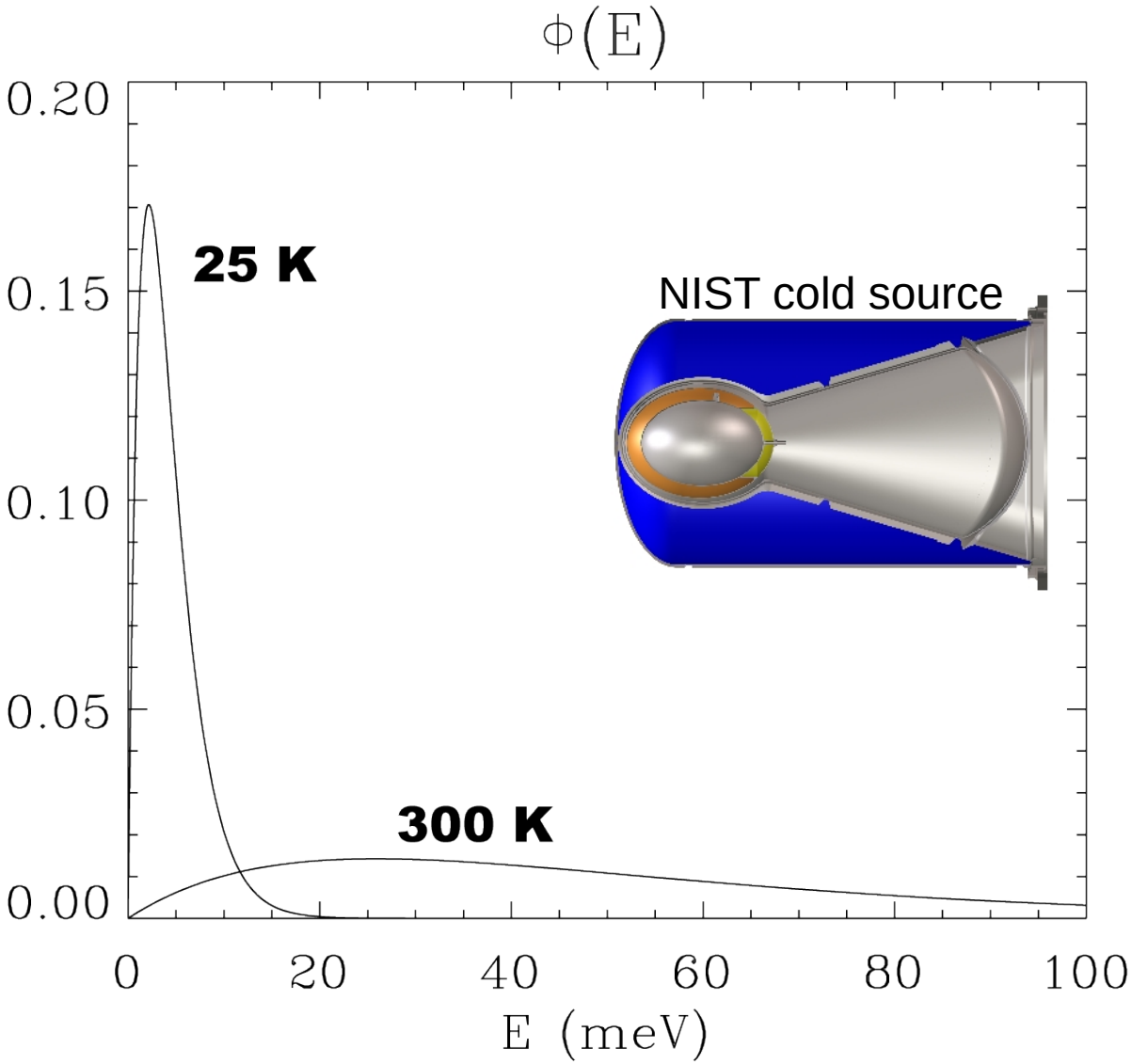
$$\Phi = 1.5 \times 10^{14}\ \mathrm{n/cm^2/s}$$

at mid-plane
(un-fueled region)

7 cycles/year
38 day cycles
250 days/year

NEUTRON SCATTERING FUNDAMENTALS

NEUTRON PRODUCTION

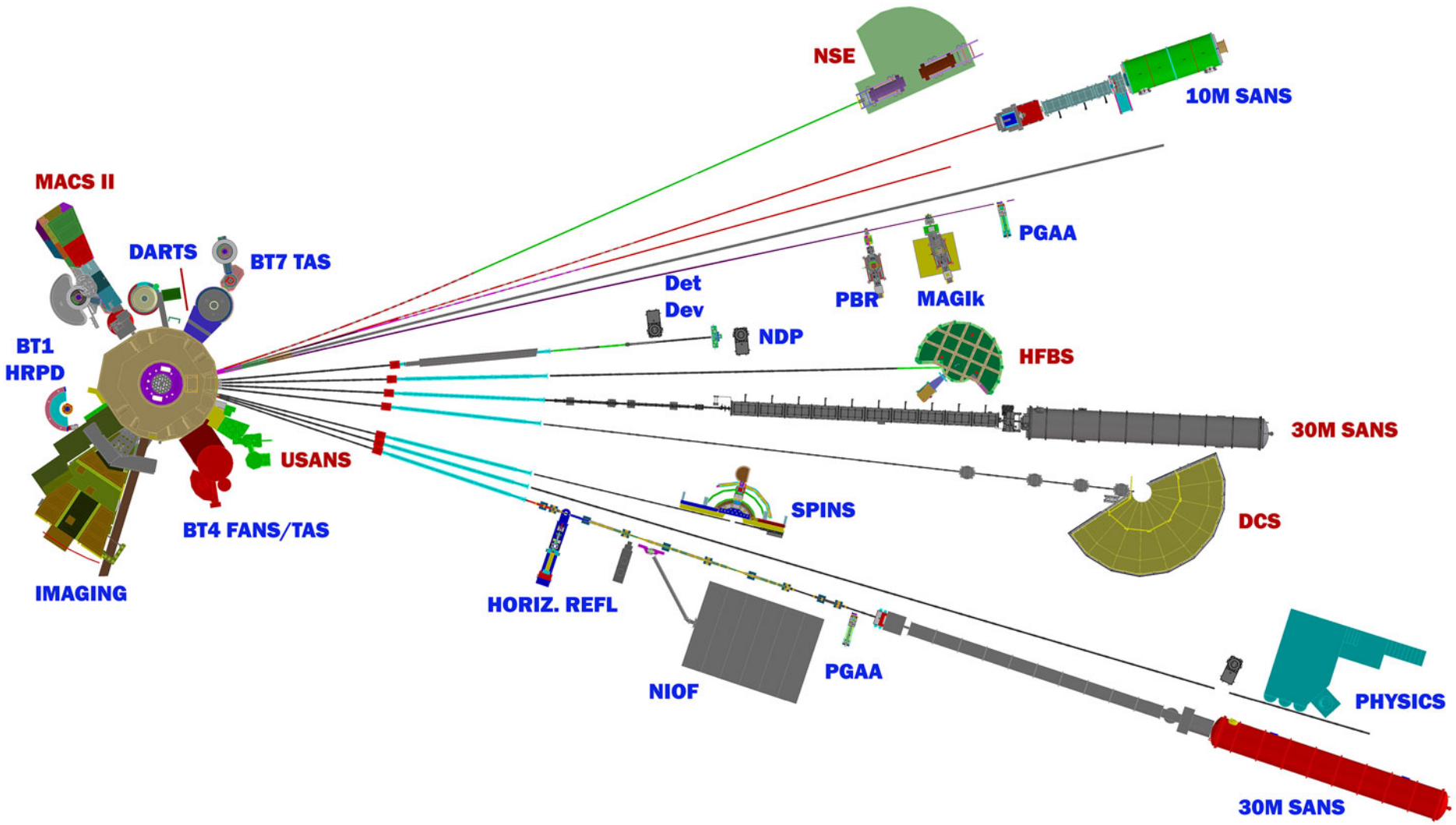


Cold neutrons (long λ, small E) are well-suited for probing structure and dynamics of soft matter such as polymers and biomolecules.

28 instruments

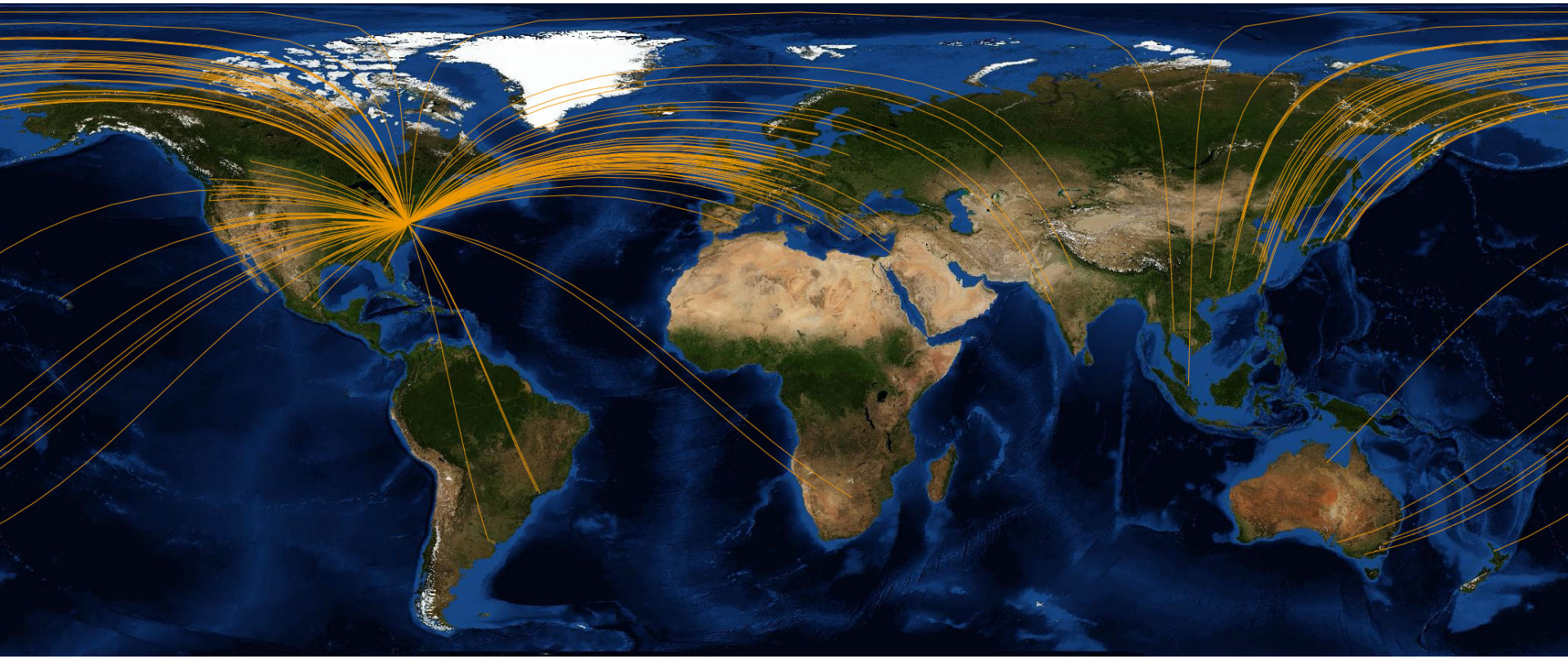
250 operating days

2 proposal calls/year

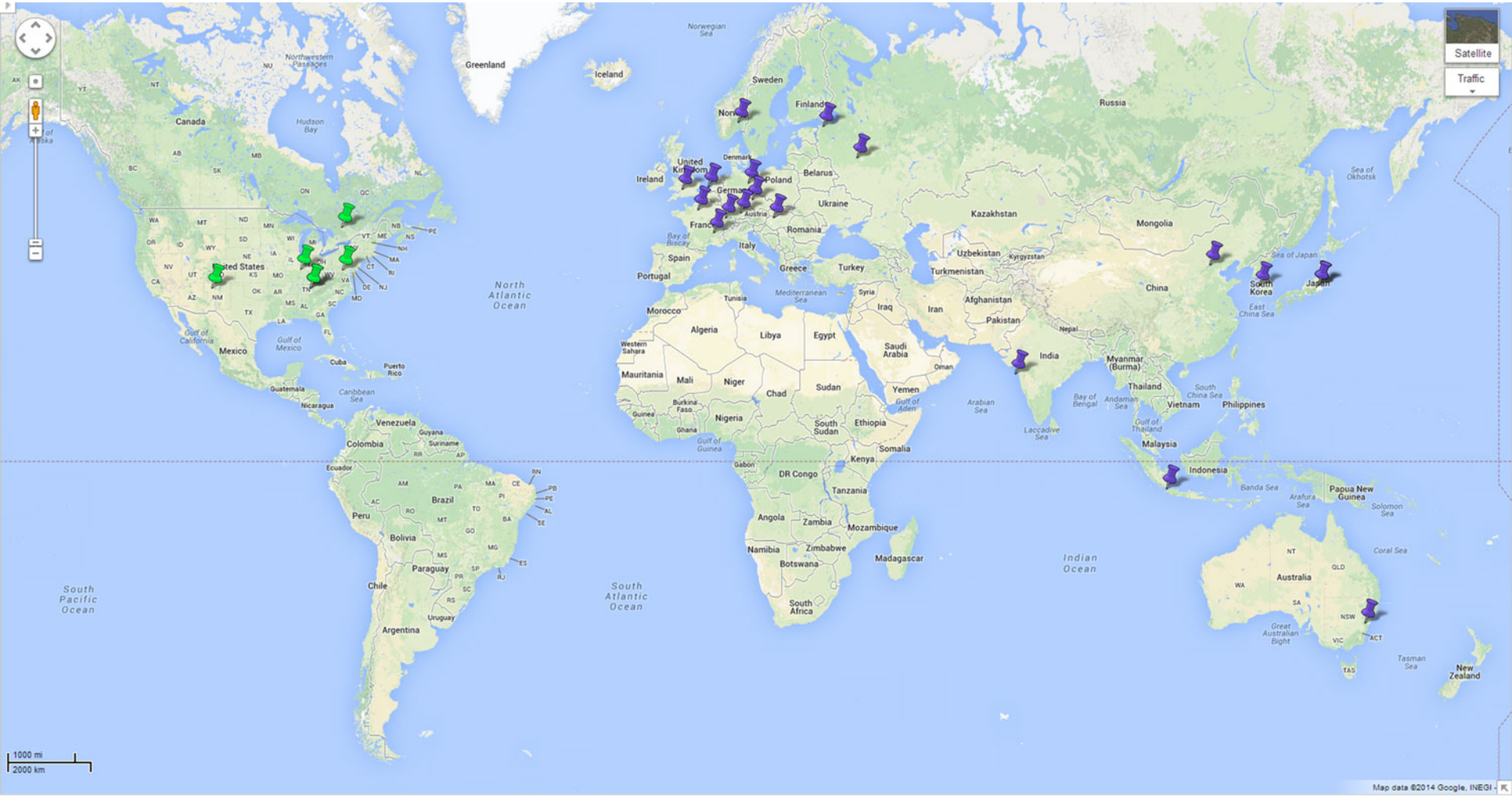


Unique instruments to address the needs of the scientific community

2013 NCNR RESEARCH PARTICIPANTS

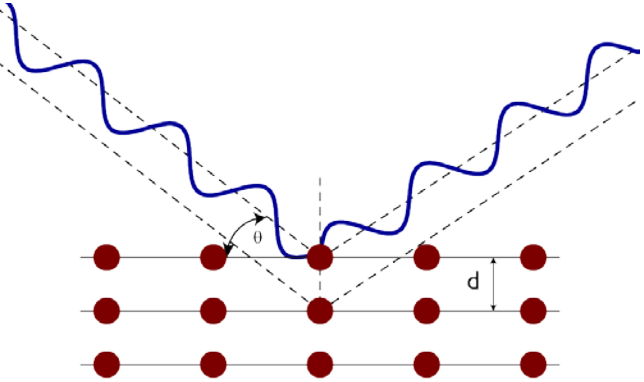


NEUTRON SCATTERING FACILITIES

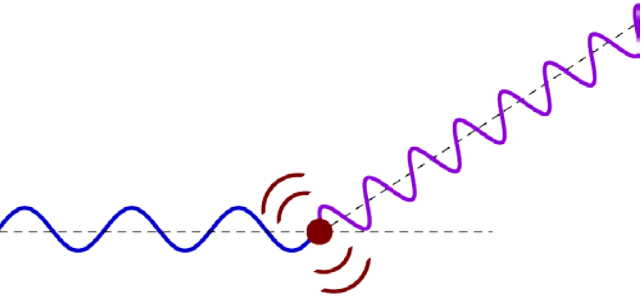


WHY NEUTRON SCATTERING?

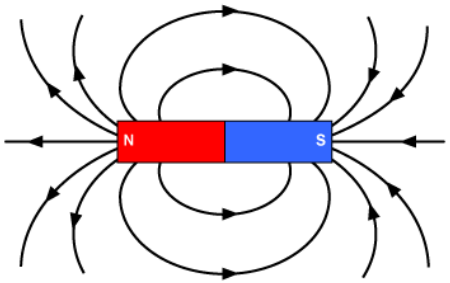
λ ~ interatomic spacing



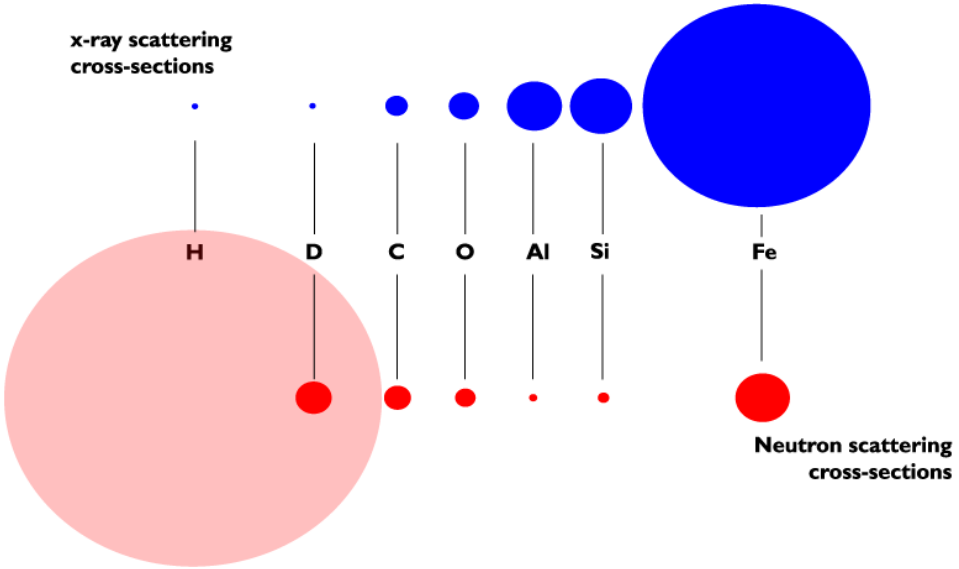
E ~ atomic motion



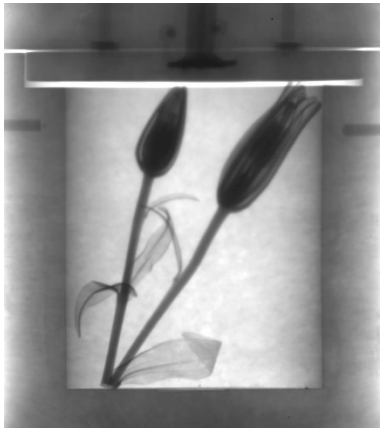
Magnetic

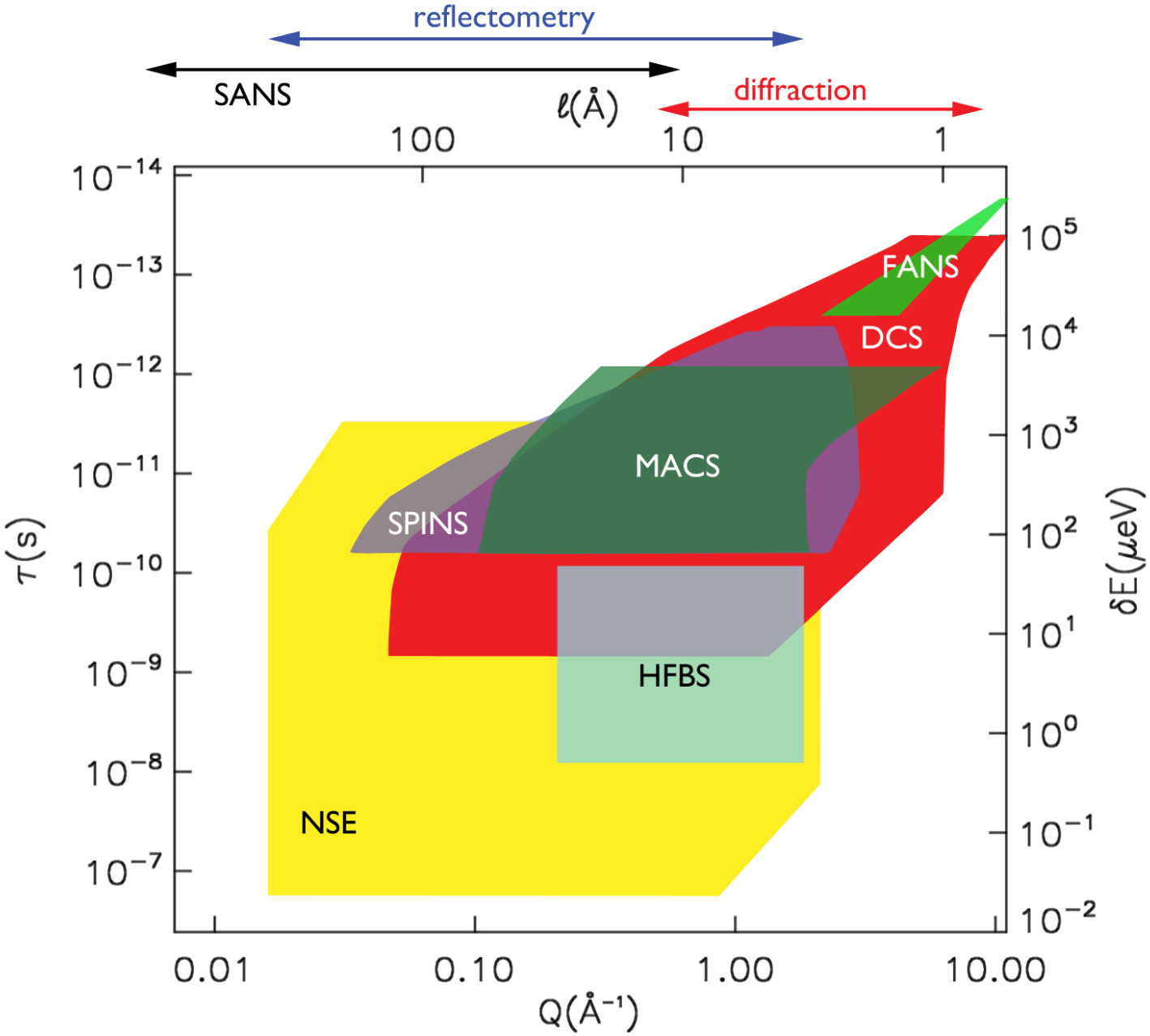


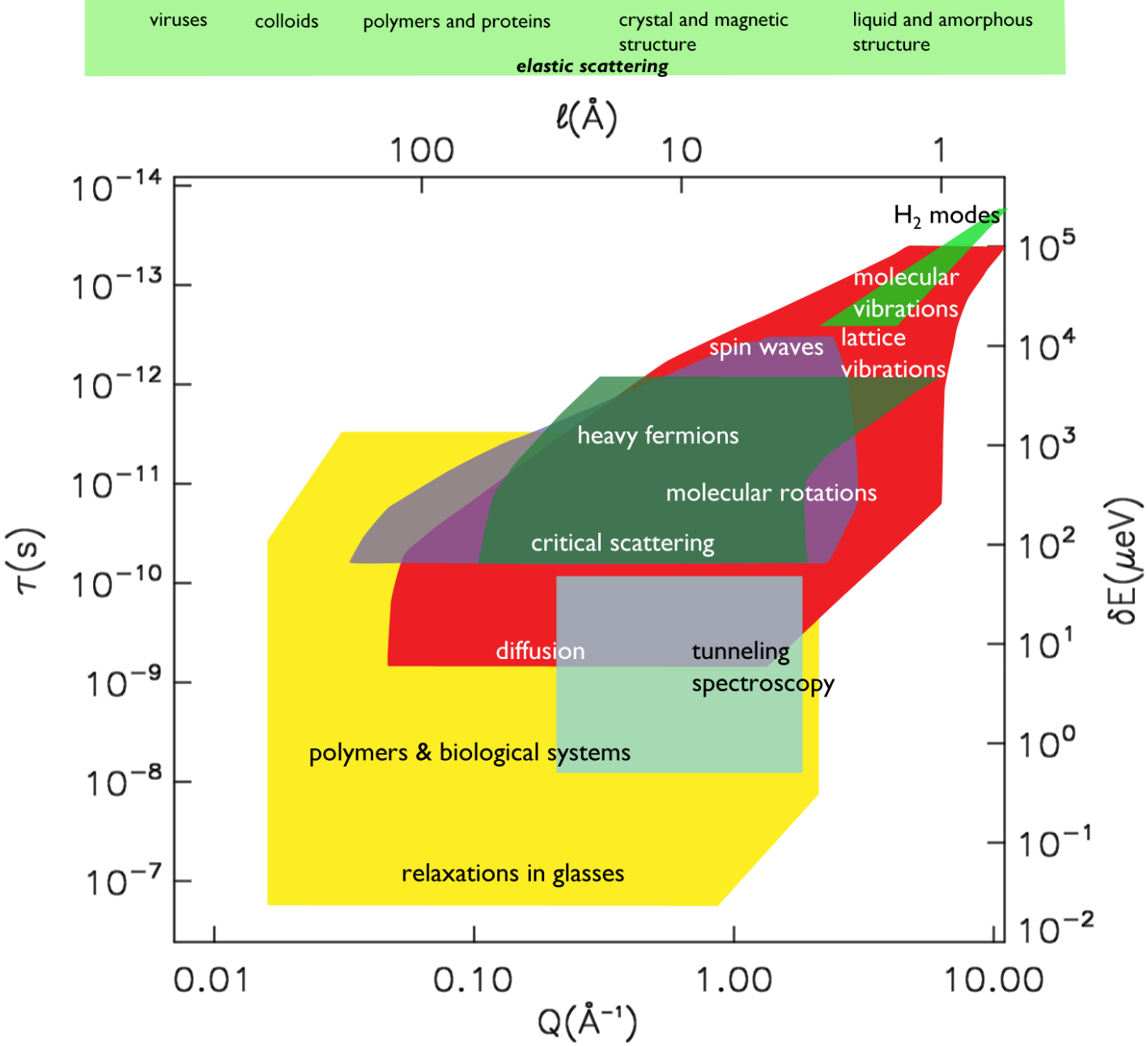
Scattering power varies randomly across the periodic table and from isotope to isotope



Penetrating

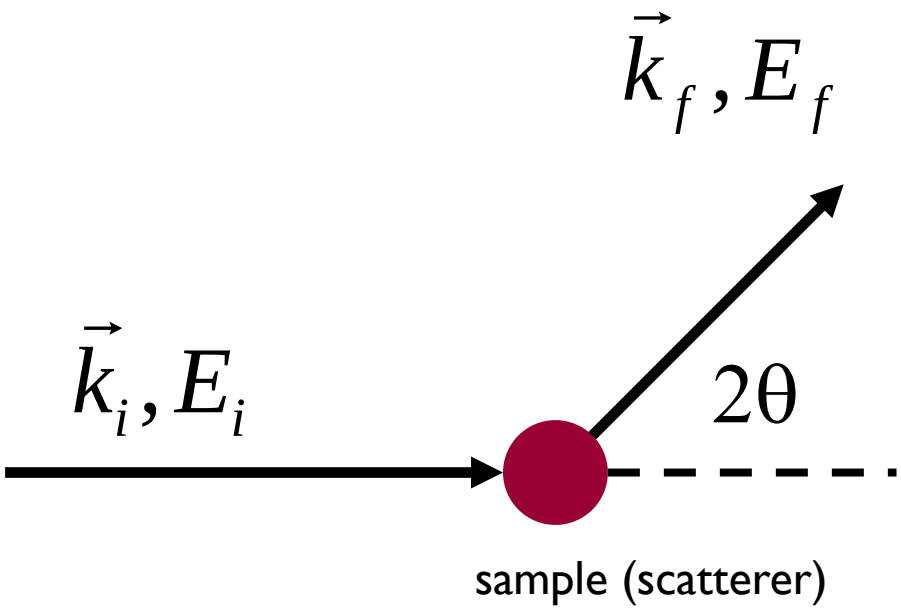



reflectometry
SANS
diffraction
ℓ(Å)
100
10
1
FANS
DCS
MACS
SPINS
HFBS
NSE
τ(s)
δE(μeV)
Q(Å⁻¹)
0.01
0.10
1.00
10.00


viruses
colloids
polymers and proteins
crystal and magnetic structure
liquid and amorphous structure
elastic scattering
ℓ(Å)
100
10
1
10^{-14}
10^{-13}
10^{-12}
10^{-11}
10^{-10}
10^{-9}
10^{-8}
10^{-7}
τ(s)
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
δE(μeV)
H_2 modes
molecular vibrations
lattice vibrations
spin waves
heavy fermions
molecular rotations
critical scattering
diffusion
tunneling spectroscopy
polymers & biological systems
relaxations in glasses
0.01
0.10
1.00
10.00
Q(Å⁻¹)

NEUTRON SCATTERING FUNDAMENTALS

KINEMATICS



$$\vec{p} = \hbar\vec{k}$$

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

$$E = E_i - E_f$$

$$E_i = \frac{(\hbar k_i)^2}{2m_n}$$

$$k^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$

NEUTRON SCATTERING FUNDAMENTALS

DYNAMICS

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma}{4\pi}\frac{k_f}{k_i} N S(\vec{Q},\omega)$$

scattering function - depends on sample properties only

$$S_{coh}(\vec{Q},\omega) = \frac{1}{2\pi\hbar N}\int \mathrm{dt}\, e^{-i\omega t}\left\langle \rho_{\vec{Q}}(0)\rho_{-\vec{Q}}(t)\right\rangle$$

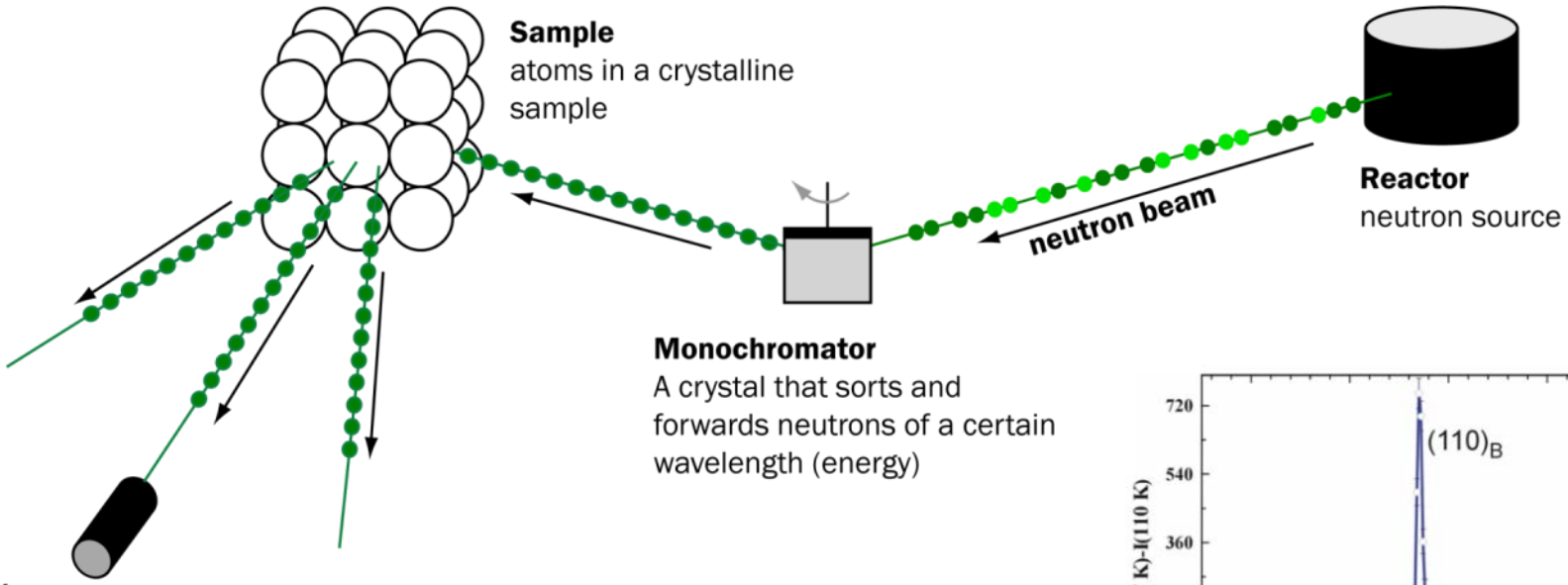
related to pair correlation function

$$S_{inc}(\vec{Q},\omega)$$

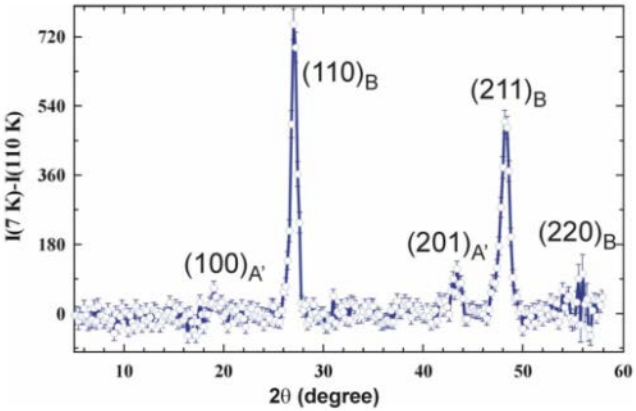
related to self correlation function

DIFFRACTION
where are the atoms?

When the neutrons collide with the atoms they change direction - they are scattered elastically.

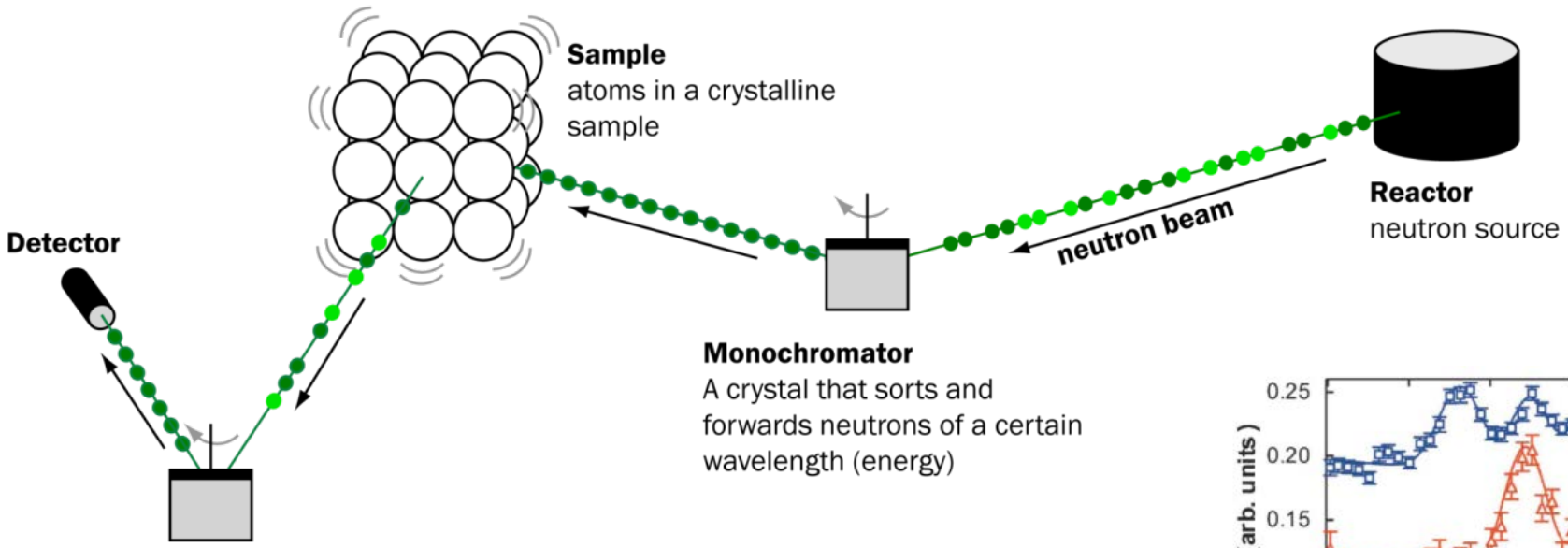


Detector
Records the directions of the neutrons and a diffraction pattern is obtained. The pattern shows the positions of the atoms relative to one another

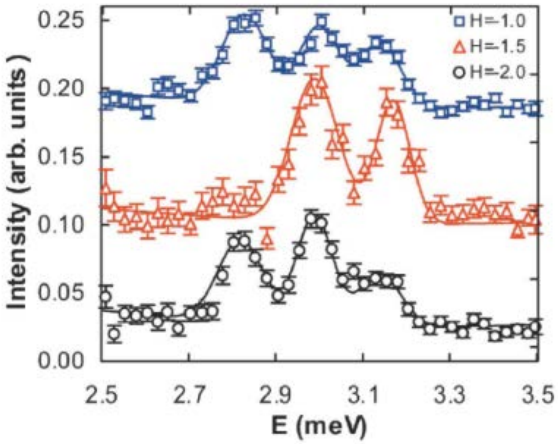


SPECTROSCOPY
how are they moving?

When the neutrons collide with the atoms, they may gain or lose energy to the atoms (inelastic scattering).

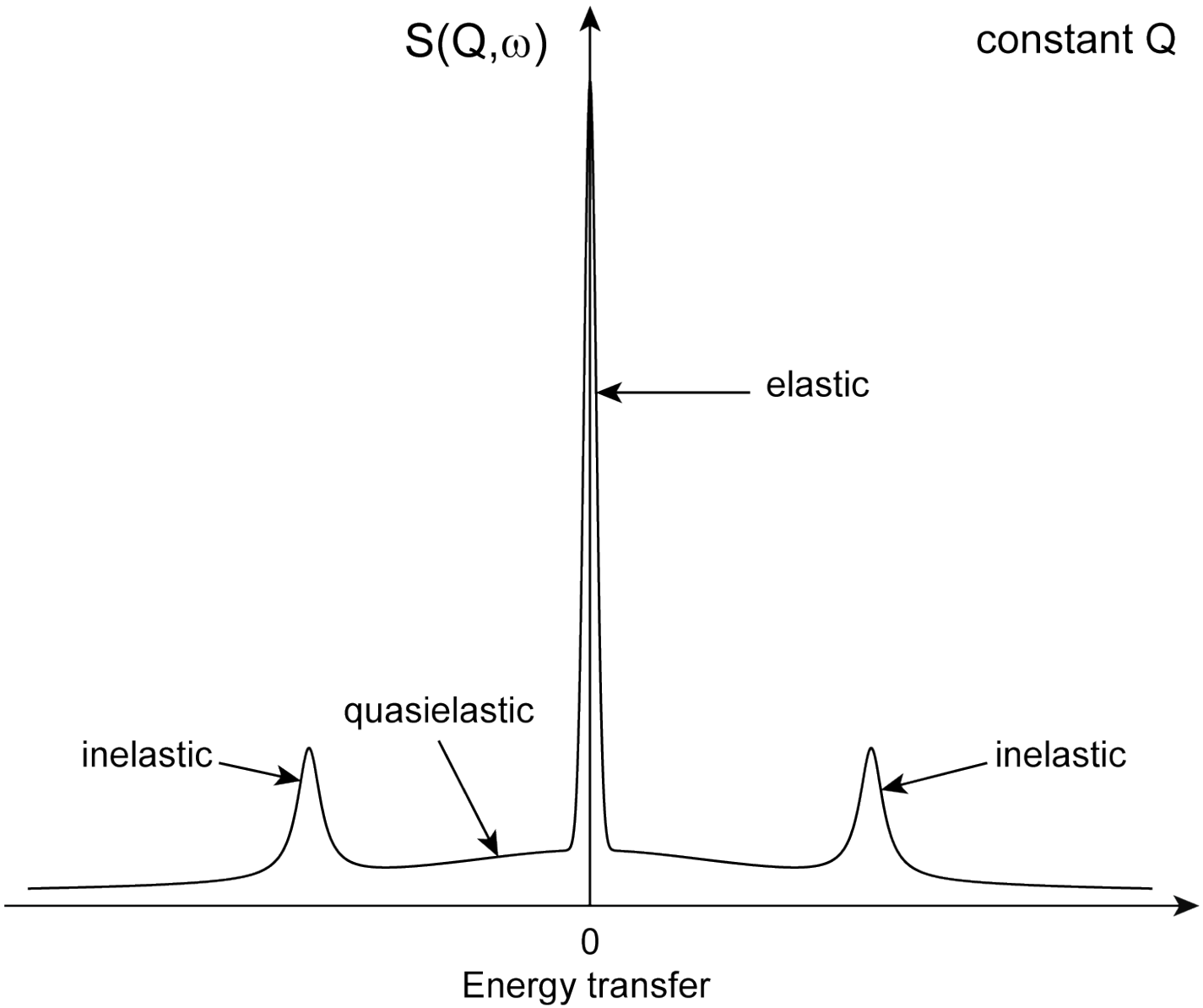


Analyzer
A crystal that sorts and forwards to the detector neutrons that have exchanged energy with the sample by a specific amount



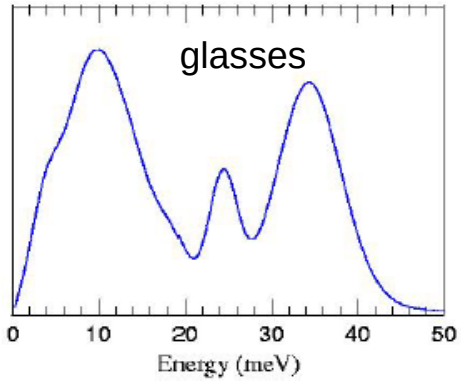
NEUTRON SCATTERING FUNDAMENTALS

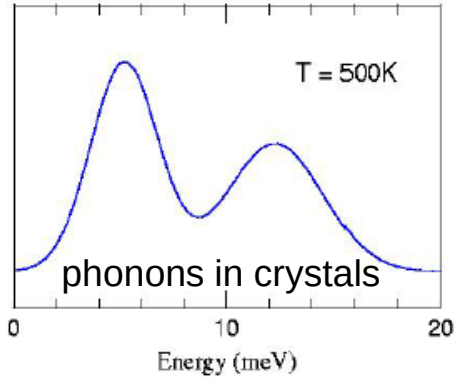
NEUTRON SPECTROSCOPY *in a nutshell*

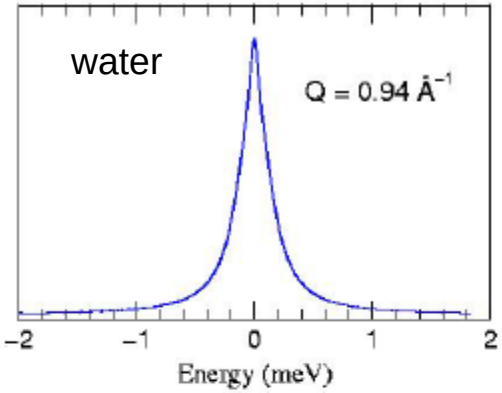


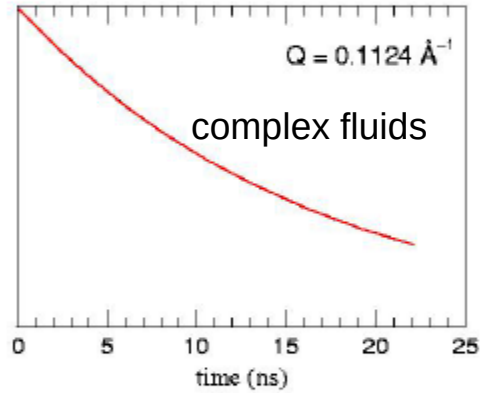
NEUTRON SCATTERING FUNDAMENTALS

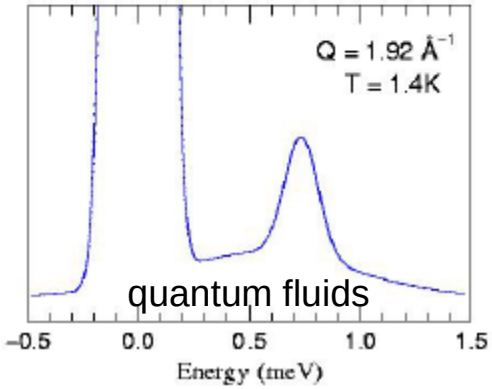
NEUTRON SPECTROSCOPY *in a nutshell*

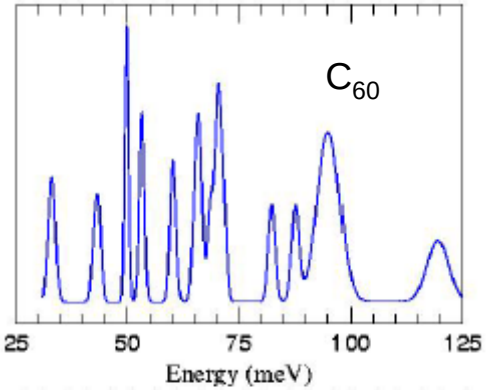


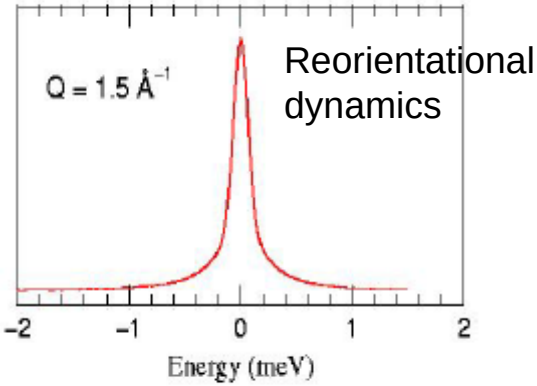


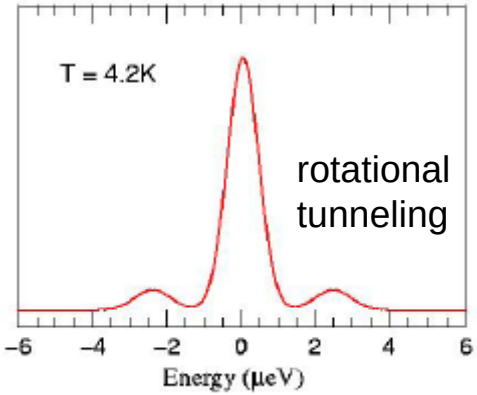






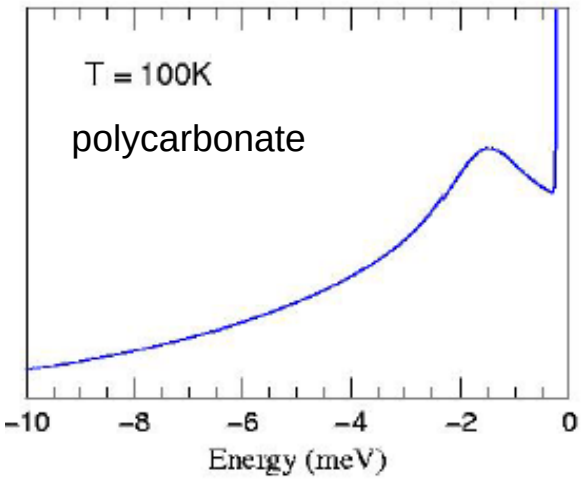


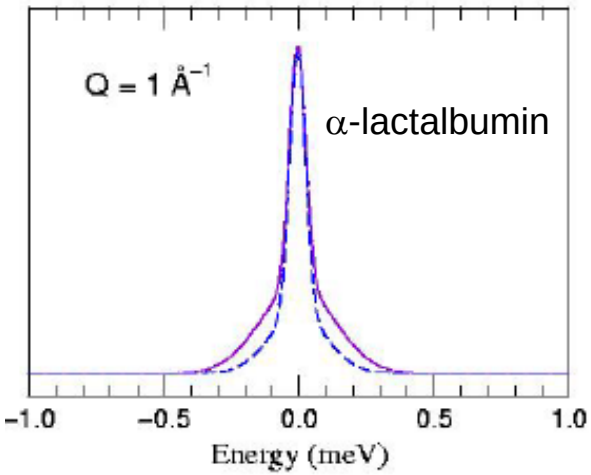


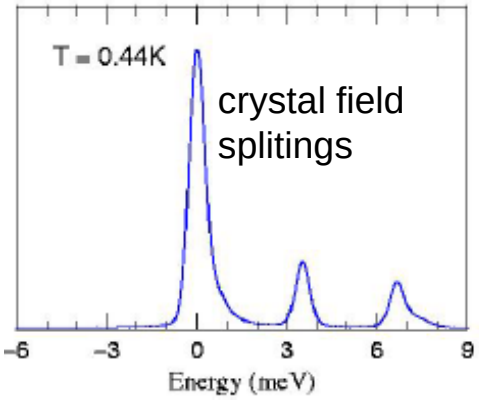


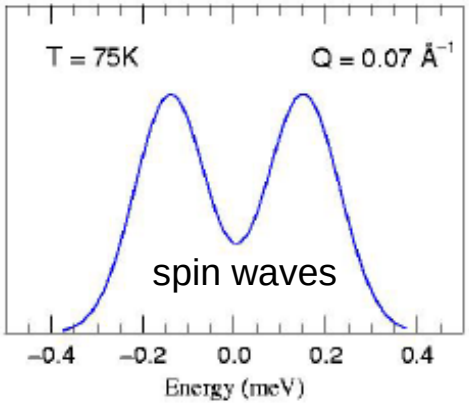
NEUTRON SCATTERING FUNDAMENTALS

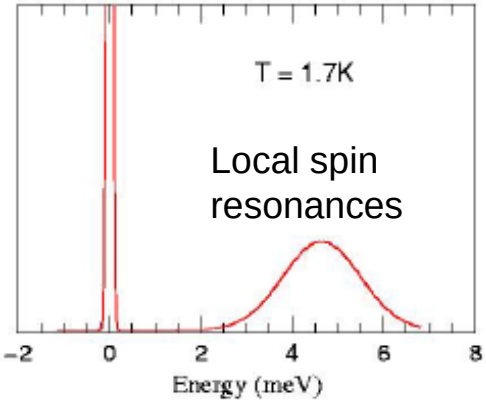
NEUTRON SPECTROSCOPY *in a nutshell*









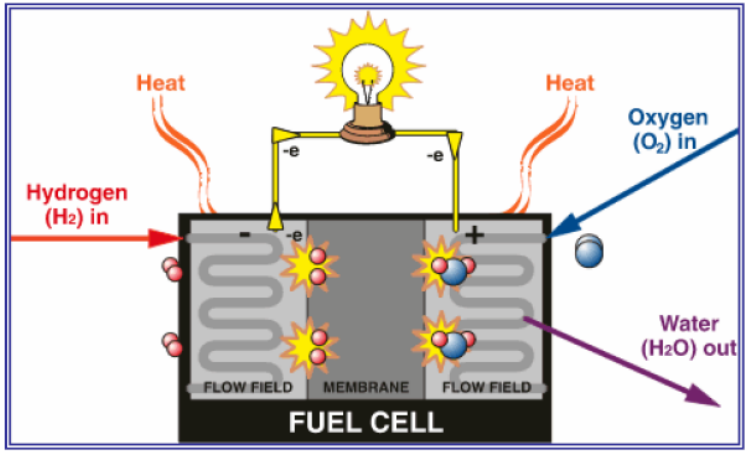


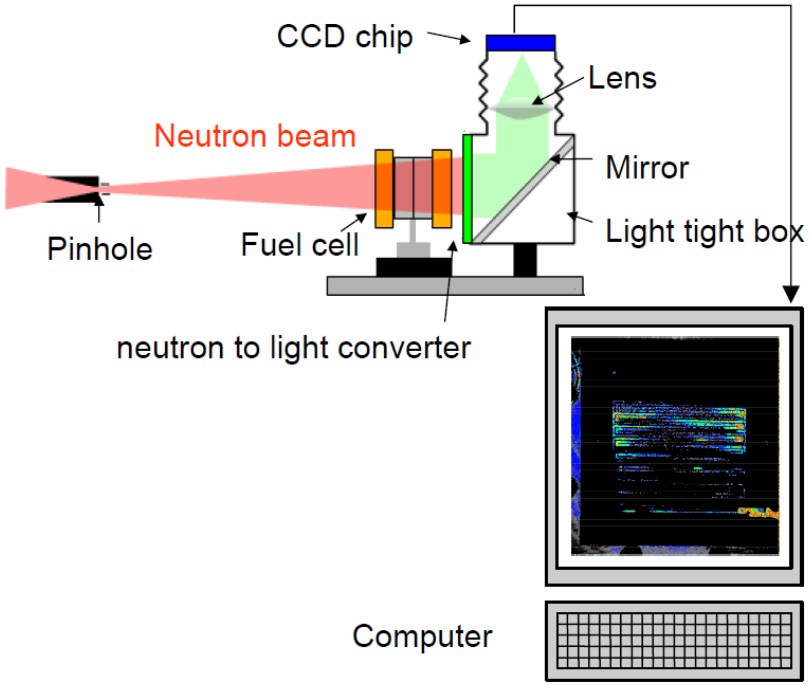
Neutron Imaging

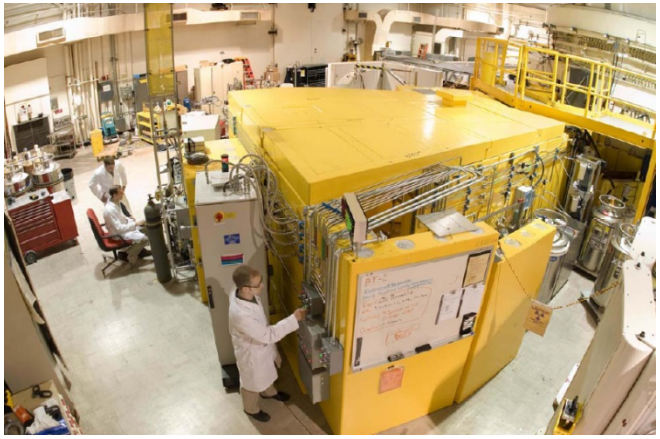
Viewing Operational Fuel Cells in Real-Time

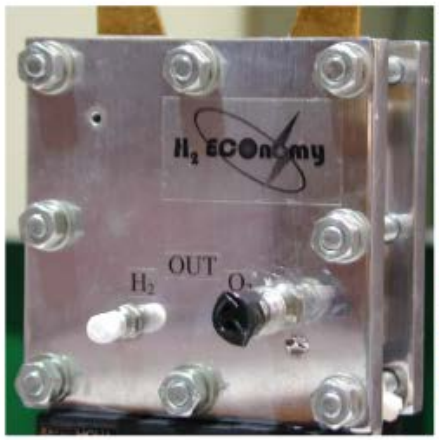
Problem: Water management in fuel cell; metal cell components; scattering from hydrogen

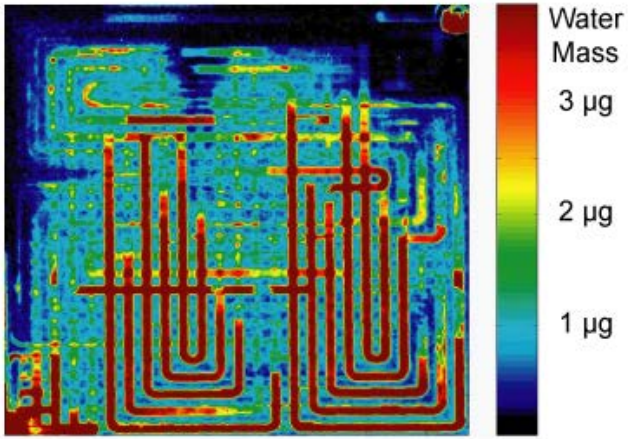
Solution: Neutron imaging







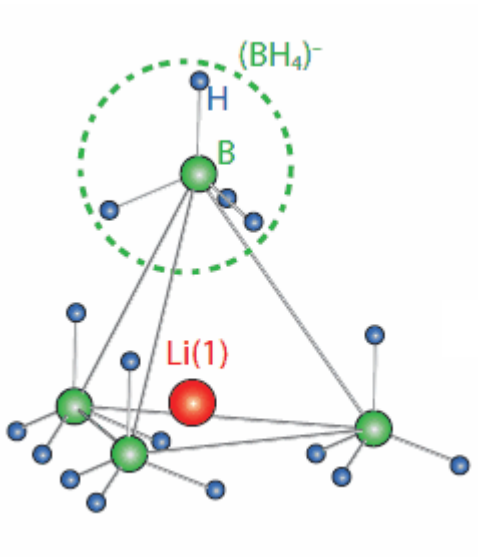


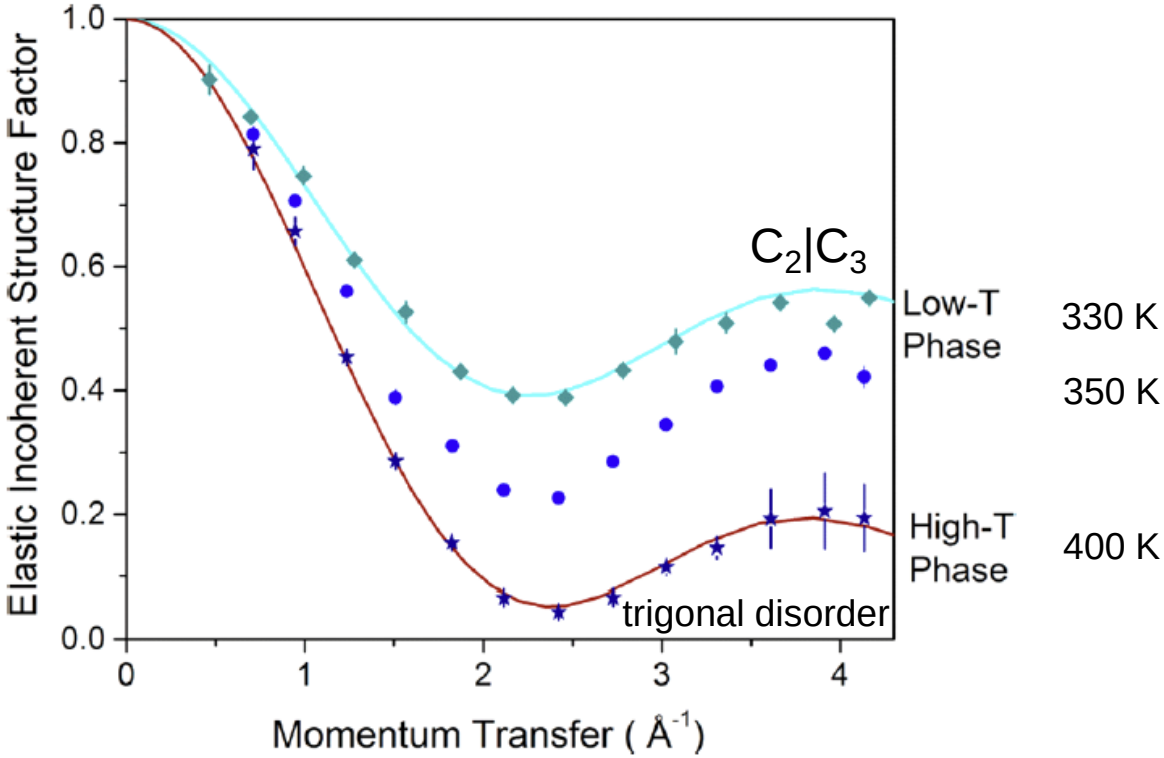


REORIENTATIONAL DYNAMICS IN NANOCONFINED $LiBH_4$

REORIENTATIONAL DYNAMICS IN NANOCONFINED $LiBH_4$

Bulk $LiBH_4$ dynamics

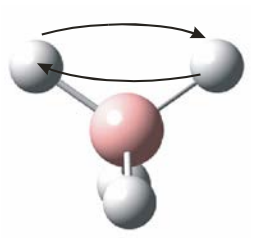




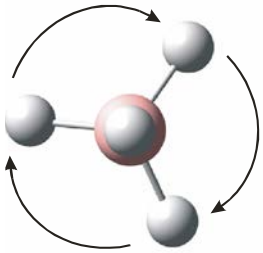
$$S(Q,\omega) = A_0(Q)\delta(\omega) + \sum_i A_i(Q)L_i(\omega)$$

$$A_0(Q) = \frac{1}{2}[1 + j_0(Qd_{H-H})]$$ $C_2|C_3$

$$A_0(Q) = j_0^2(Qd_{H-H})$$



two-fold jumps

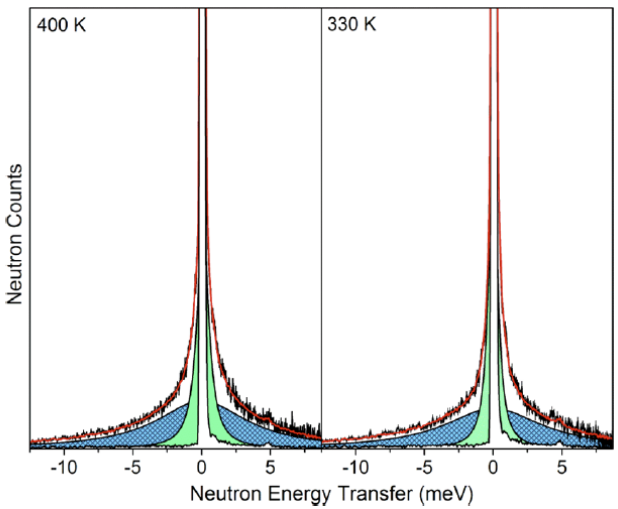


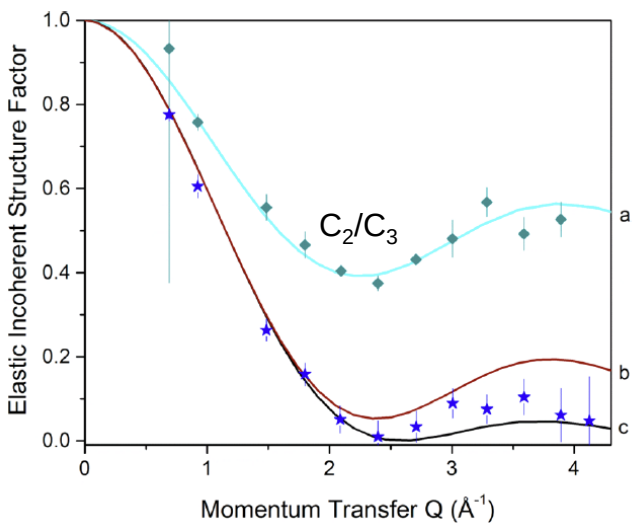
three-fold jumps

Verdal et. al., J. Phys. Chem. C **117** (35) 17983 (2013)

REORIENTATIONAL DYNAMICS IN NANOCONFINED $LiBH_4$

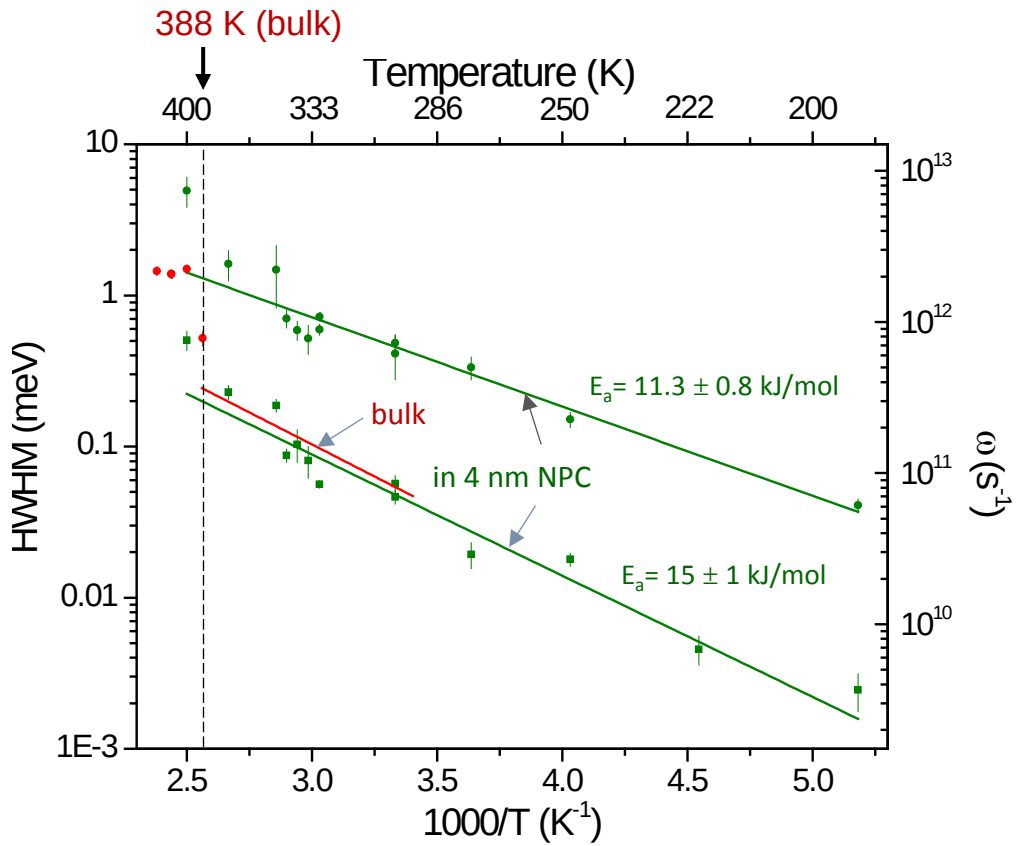
$LiBH_4$ in NPC-4 nm





330 K

400 K Isotropic rotational diffusion



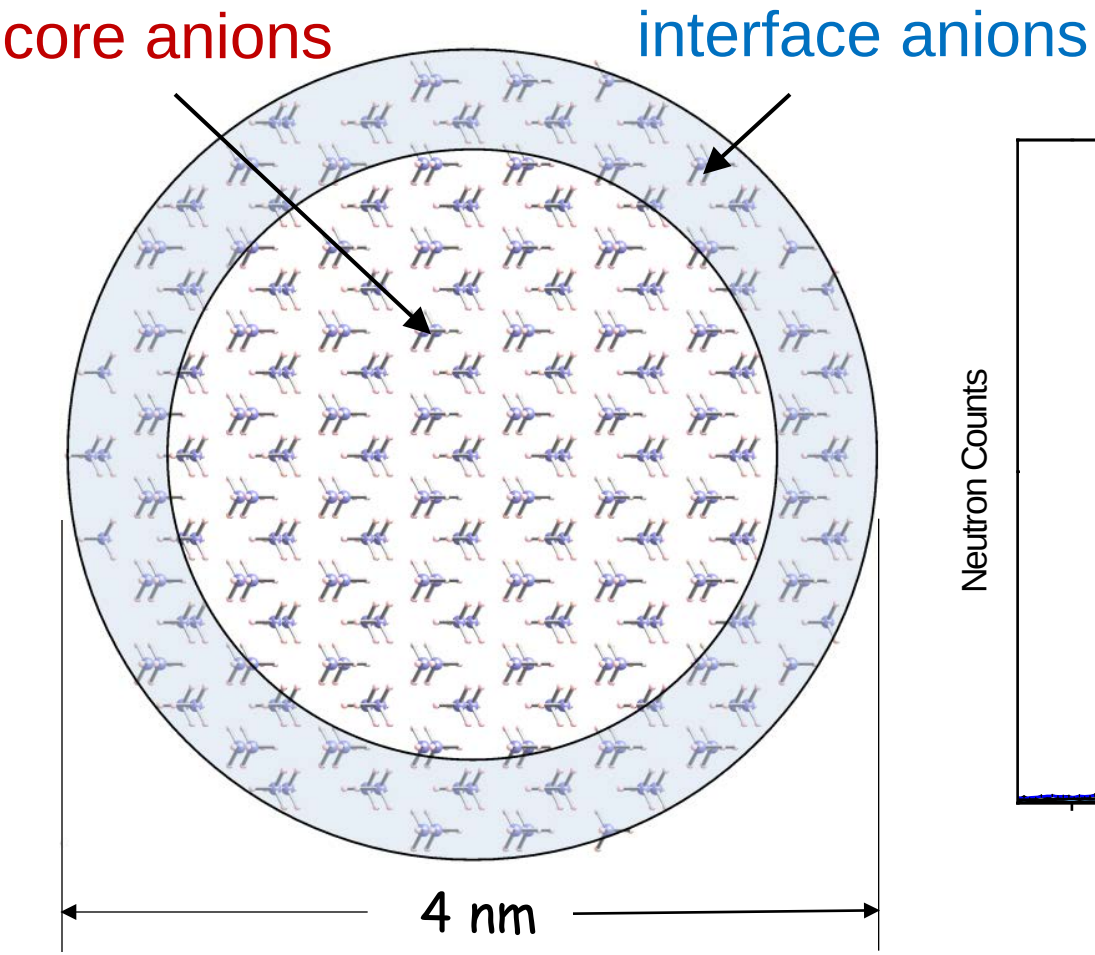
Verdal et. al., J. Phys. Chem. C **117** (35) 17983 (2013)

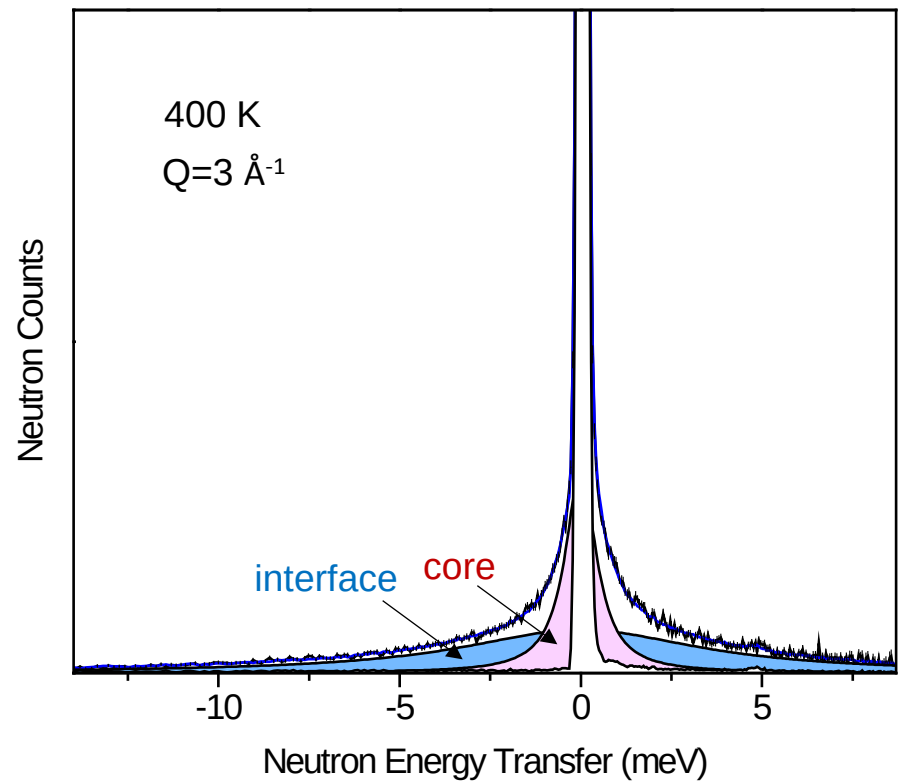
REORIENTATIONAL DYNAMICS IN NANOCONFINED $LiBH_4$

two types of BH_4^- anions in 4 nm cylindrical pores

core BH_4^- anions with slower, bulk-like, jump reorientations

interface BH_4^- anions with faster, more disordered reorientations



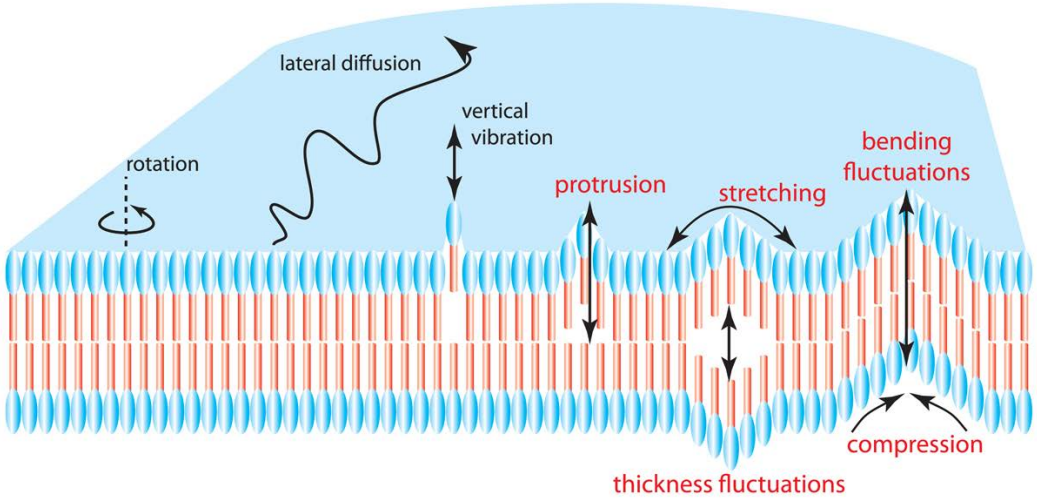


Verdal et. al., J. Phys. Chem. C **117** (35) 17983 (2013)

THICKNESS FLUCTUATIONS IN CELL MEMBRANES

THICKNESS FLUCTUATIONS IN CELL MEMBRANES

Do thickness fluctuations in biological membranes exist and do they form pores thus allowing proteins to work their way inside?



Requires measurements of longer time scales

$\Rightarrow$ NSE

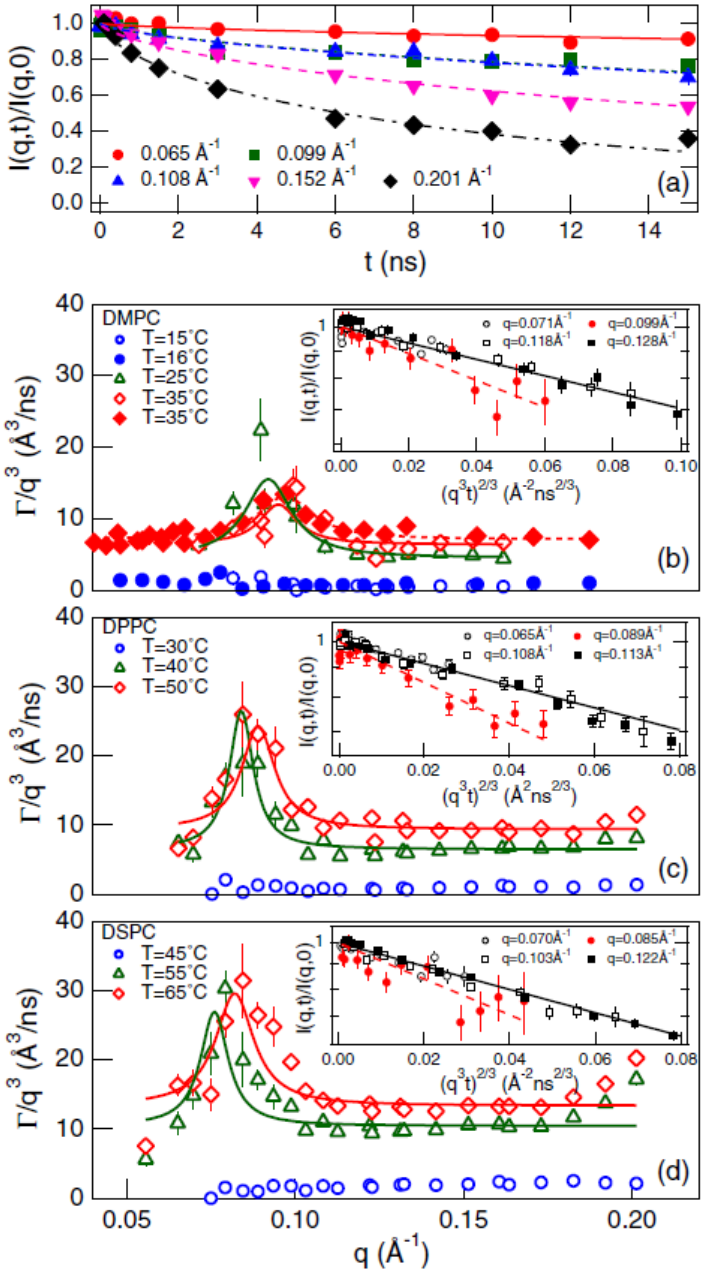
Woodka et. al., PRL **109** 058102 (2012)

THICKNESS FLUCTUATIONS IN CELL MEMBRANES

$$\frac{I(q,t)}{I(q,0)} = \exp[-(\Gamma t)^{2/3}]$$

$$\frac{\Gamma}{q^3} = \frac{\Gamma_{\mathrm{BEND}}}{q^3} + \frac{\Gamma_{\mathrm{TF}}}{q_0^3}\frac{1}{1+(q-q_0)^2\xi^{-2}}$$

$$\Gamma_{\mathrm{BEND}} = 0.025\alpha\sqrt{\frac{k_{\mathrm{B}}T}{\tilde{\kappa}}}\frac{k_{\mathrm{B}}T}{\eta_{\mathrm{D_2O}}}q^3$$



Woodka et. al., PRL **109** 058102 (2012)

THICKNESS FLUCTUATIONS IN CELL MEMBRANES

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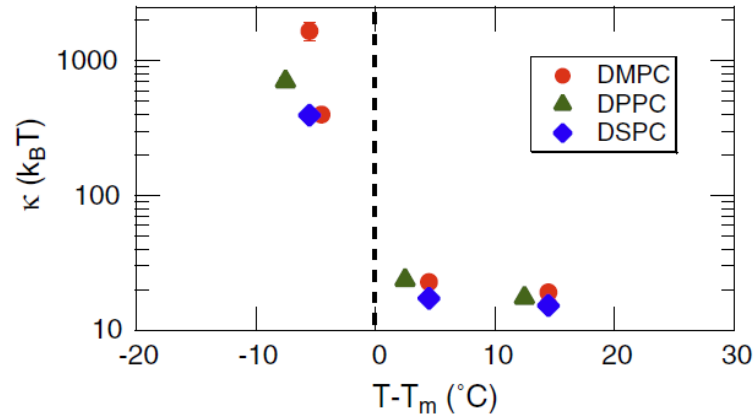
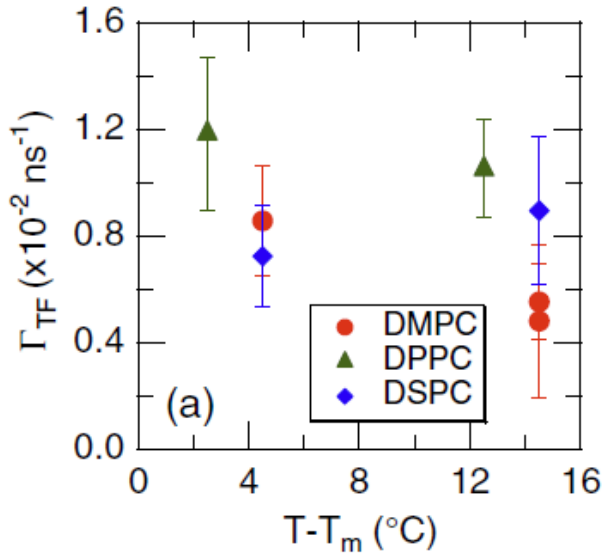
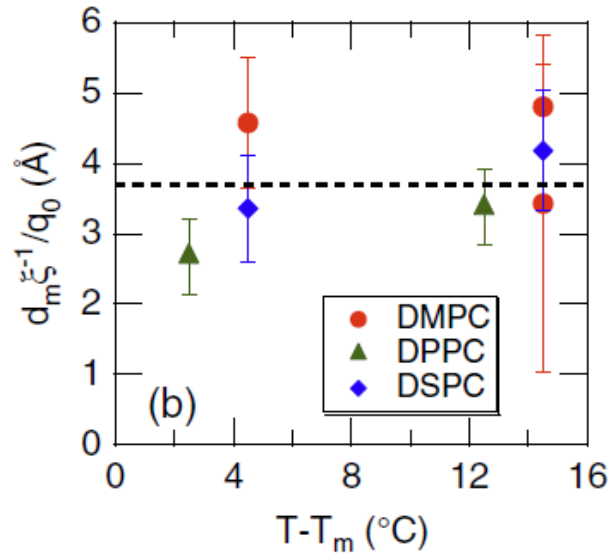






Fluctuations measured in a biological membrane for the first time directly using NSE.

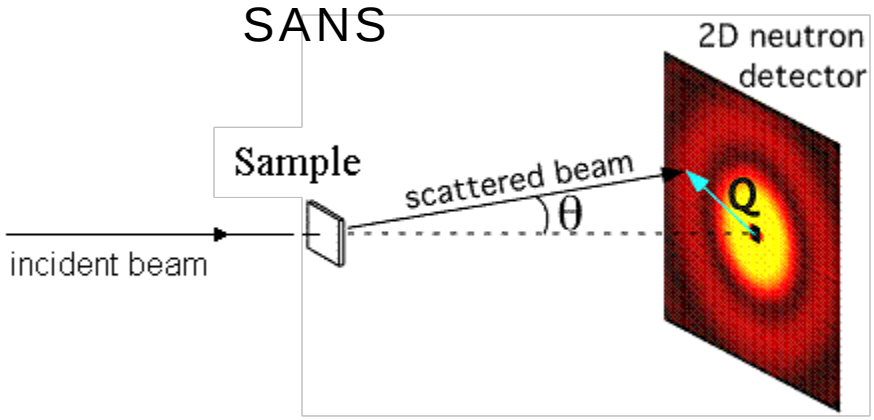
The means by which they form pores remains unsolved.

Woodka et. al., PRL **109** 058102 (2012)

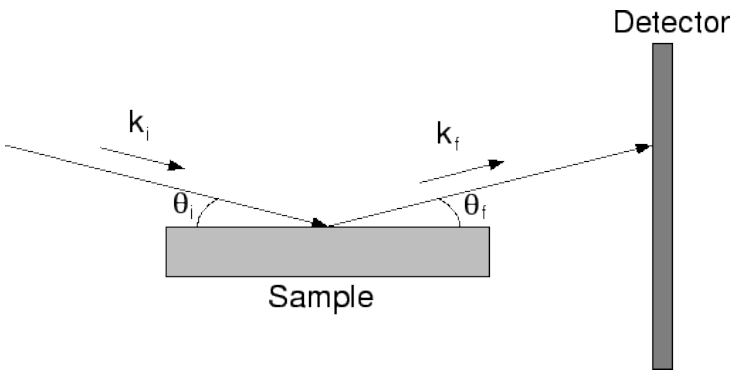
SEALING BIOMEMBRANES VIA BIO-MIMETIC POLYMERS

A structural and dynamics study

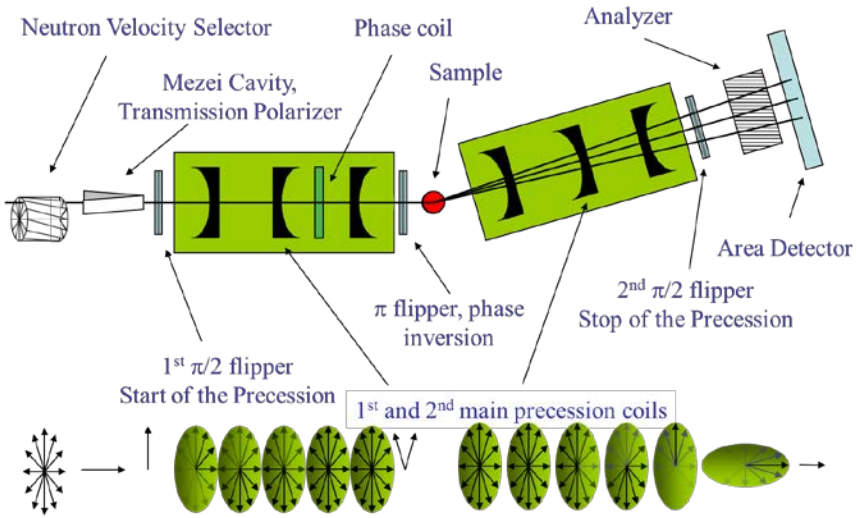
SANS



REFLECTOMETRY



NEUTRON SPIN-ECHO



SEALING BIOMEMBRANES VIA BIO-MIMETIC POLYMERS

A structural and dynamics study

Trauma can disrupt barrier function of cell membrane's barrier function

Cell repair process can be too slow resulting in dysfunction and/or damage

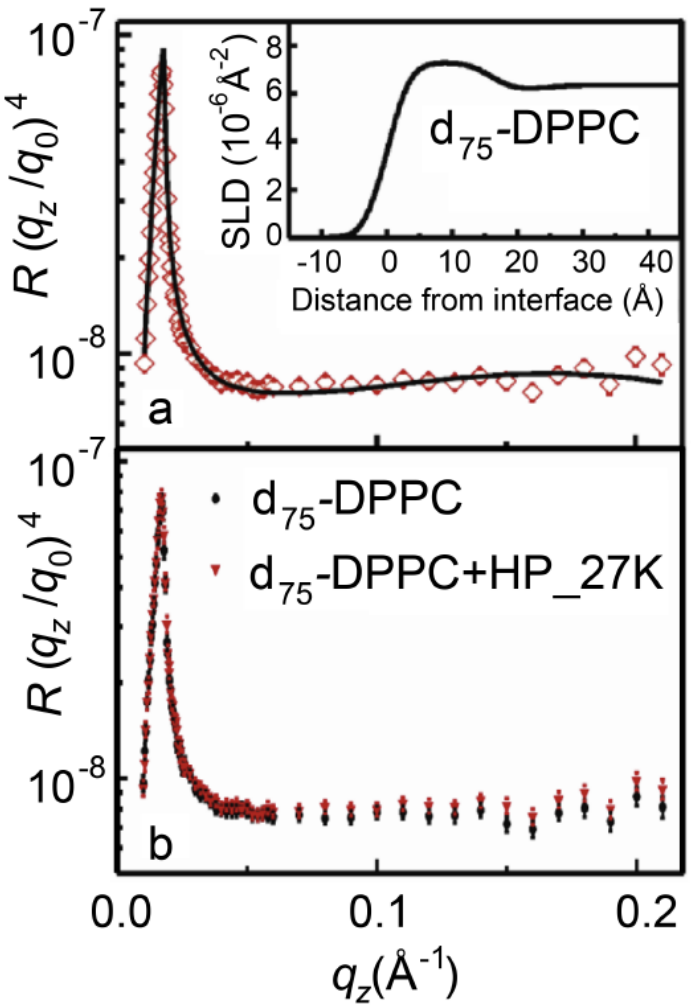
Biocompatible polymer material is a candidate for sealing the cell and enhancing cell survival

Must gain a thorough understanding of the fundamental mechanism responsible for the sealing action

J.-Y. Wang et. al., submitted

SEALING BIOMEMBRANES VIA BIO-MIMETIC POLYMERS

A structural and dynamics study



d_{75}-DPPC is a surrogate for cell membrane

1,2-dipalmytoyl (d_{62})-*sn-glycerol*-3-phosphocholine-1,1,2,2,-d_4-N,N,N-trimethyl-d_9

Sealant is a biocompatible polymer (HP_27K) with phosphorylcholine (PC) pendant groups that mimic phospholipids

Neutron Reflectometry

Head group thickness = 0.62 nm
Tail group thickness = 1.59 nm

Little difference in SLD

But at T=25 ^{o}C the high packing density might limit ability of PC polymer to interact with the lipids (which would not change the NR profile much).

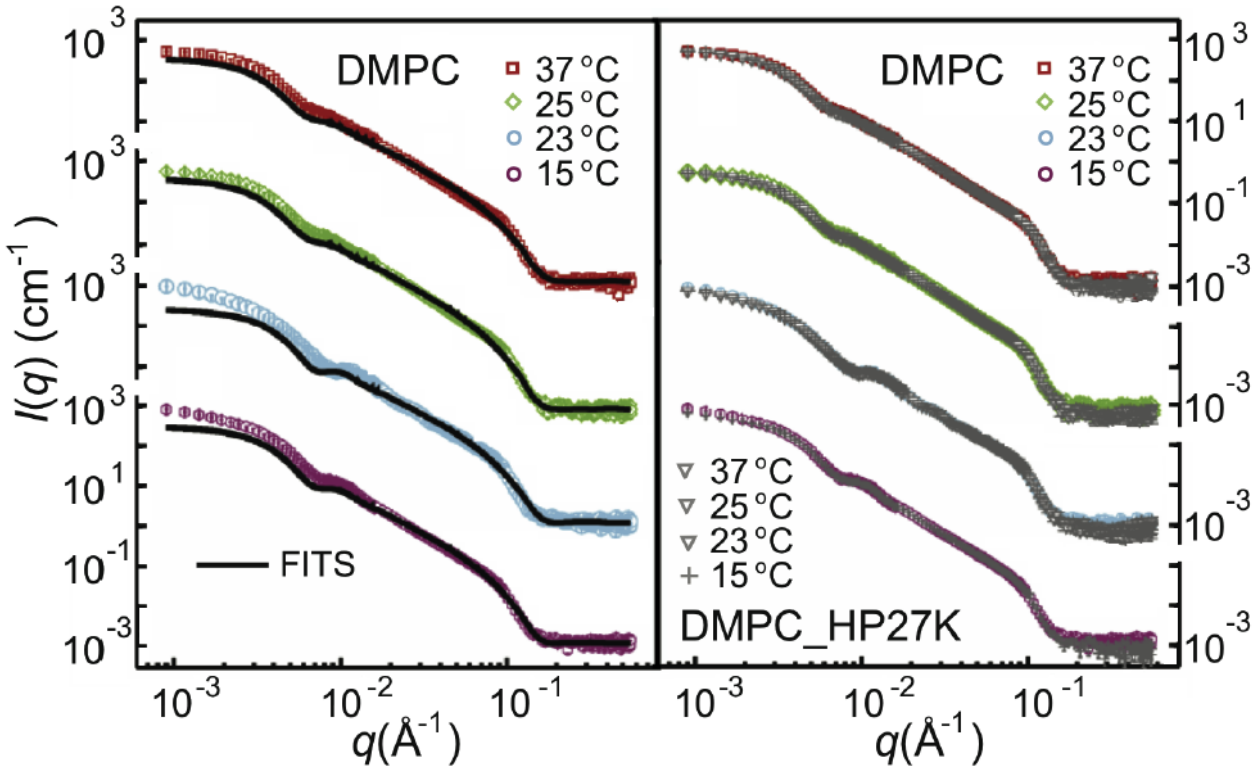
J.-Y. Wang et. al., submitted

SEALING BIOMEMBRANES VIA BIO-MIMETIC POLYMERS

A structural and dynamics study

1,2-dimyristoyl-sn-glycerol-3-phosphocholine

Small Angle Neutron Scattering



DMPC used as a surrogate for cell membrane

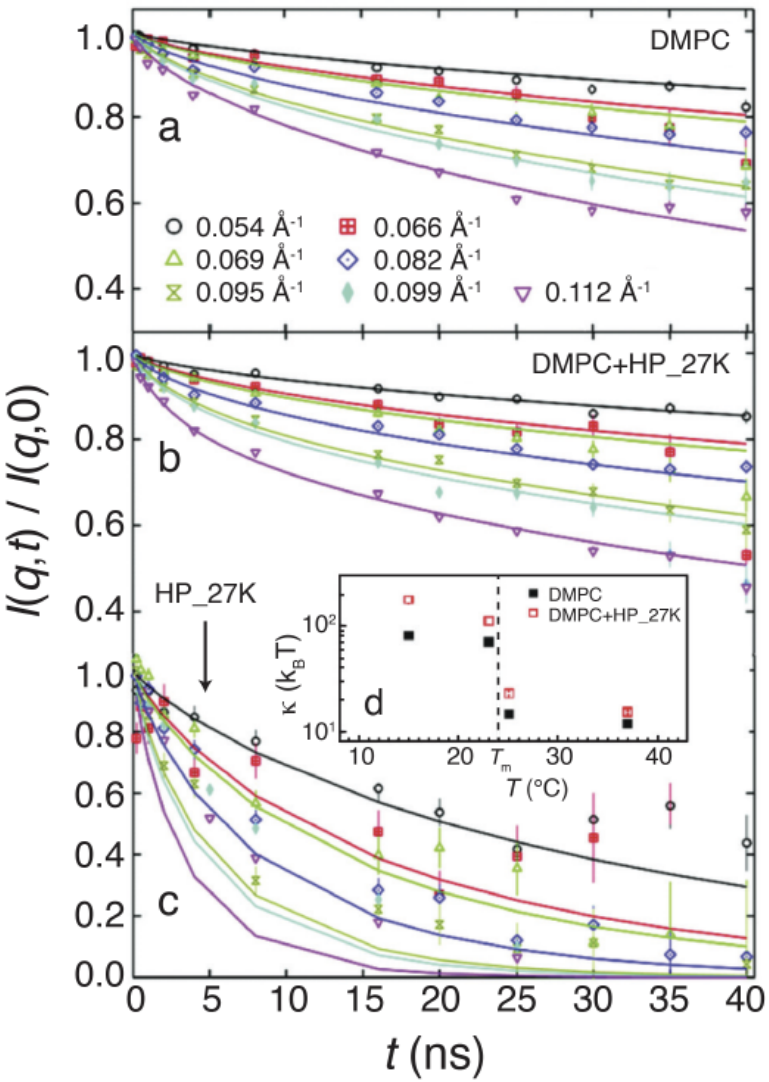
SANS measurements spanning T_m show little difference in scattering profile

Sealant has little influence on structure of lipid membranes

J.-Y. Wang et. al., submitted

SEALING BIOMEMBRANES VIA BIO-MIMETIC POLYMERS

A structural and dynamics study



J.-Y. Wang et. al., submitted

Neutron Spin Echo

DMPC used as a surrogate for cell membrane

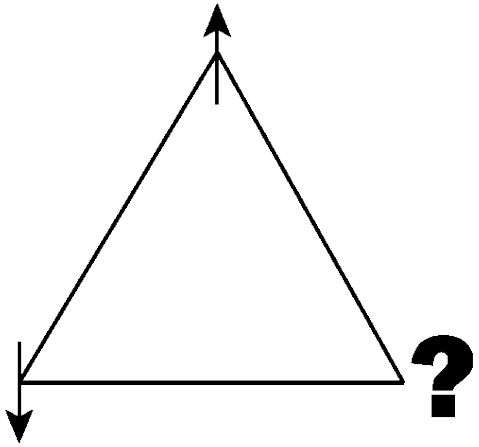
Measured membrane fluctuations

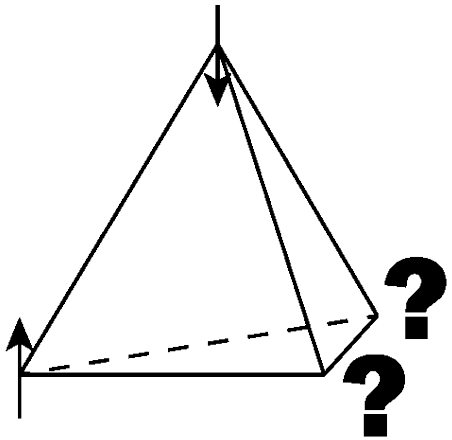
Bending modulus larger (stiffer) for system with sealant

Sealant interacts through PC-PC head groups

⇒ Sealant suppresses membrane fluctuations

QUANTUM SPIN LIQUID

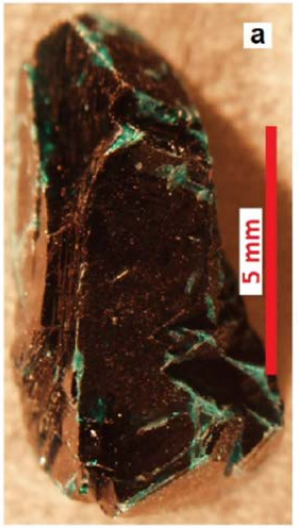


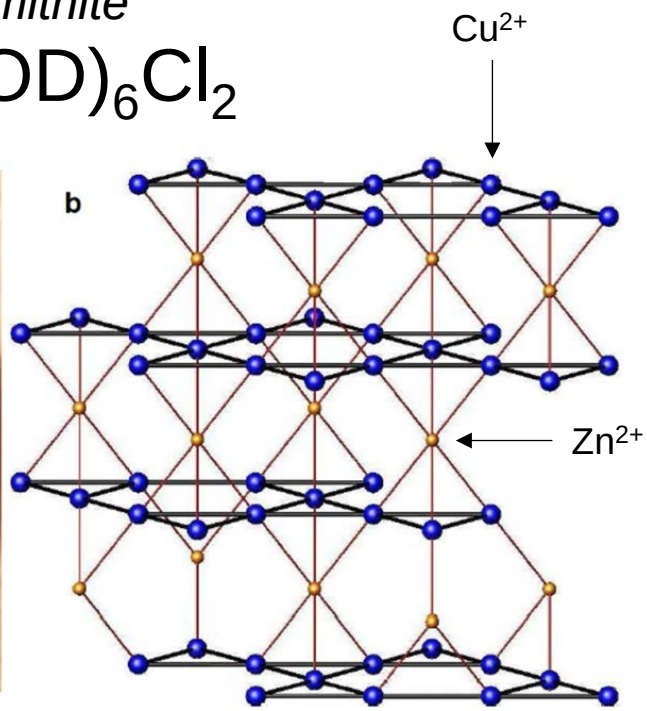


Geometric frustration
→QSL

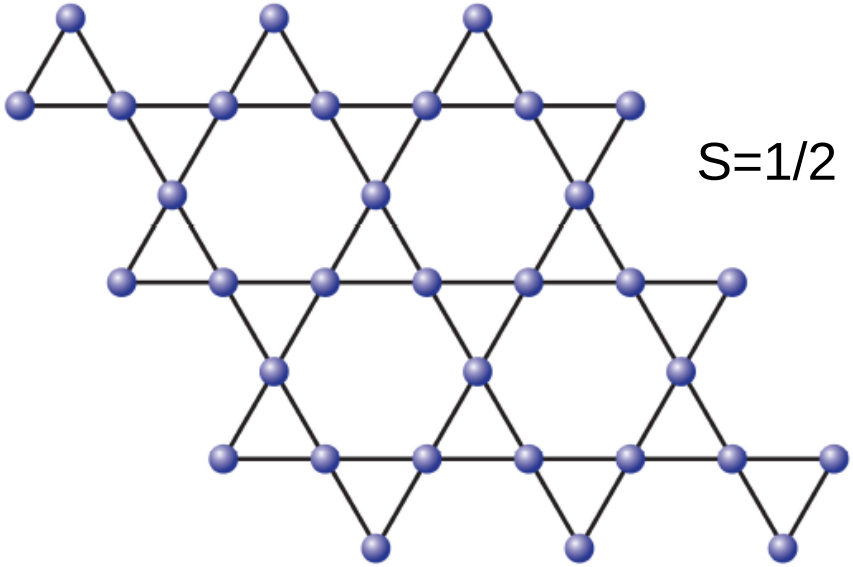
Herbertsmithite

$ZnCu_3(OD)_6Cl_2$





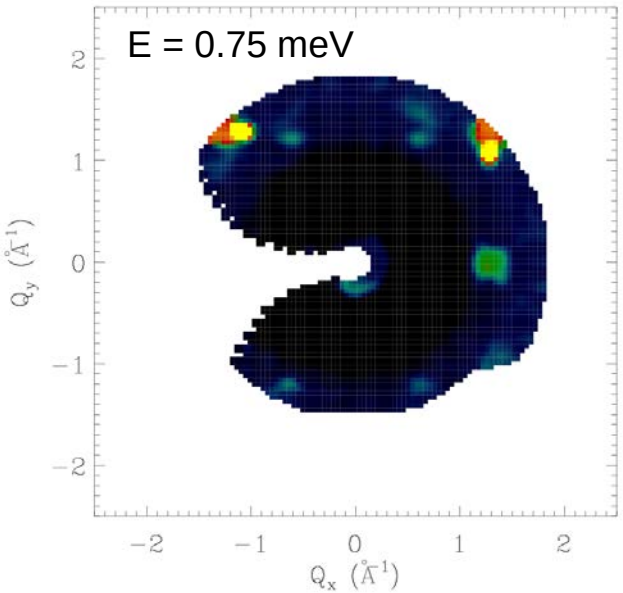
Kagome lattice antiferromagnet

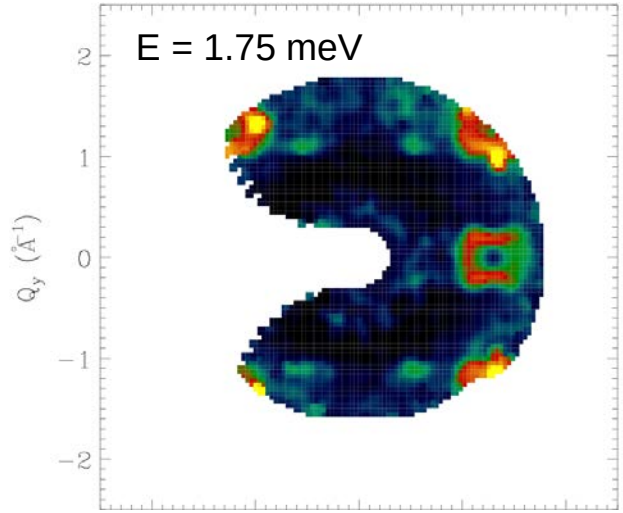


S=1/2

T.-H. Han et. al., Nature **492** 11659 (2012)

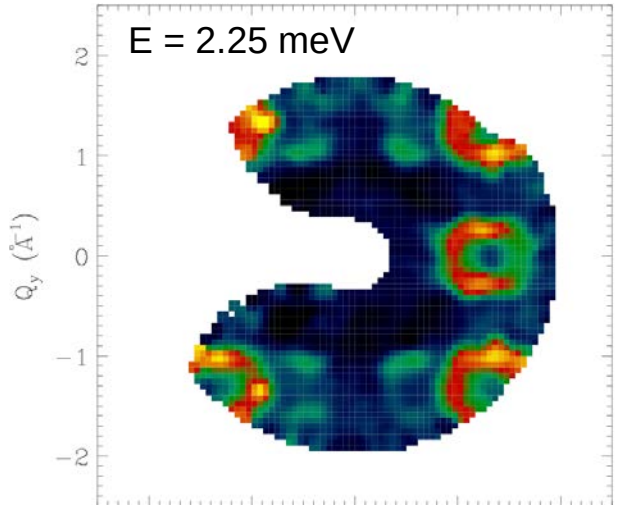
QUANTUM SPIN LIQUID...NOT

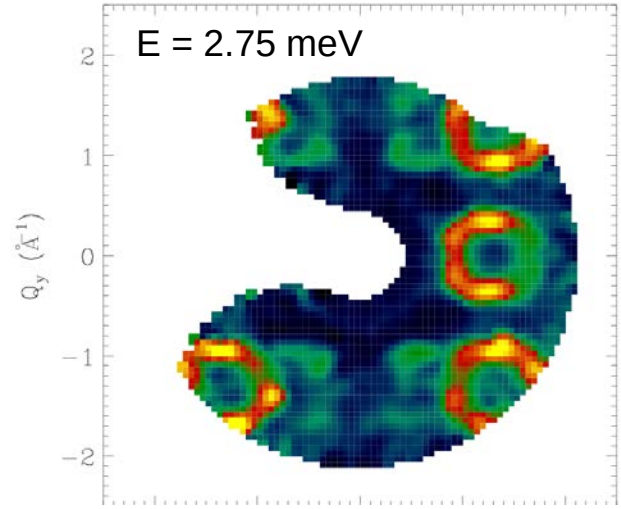




T = 2.2 K

In contrast to a quantum spin liquid, this system magnetically orders at low temperature and sharp excitations appear





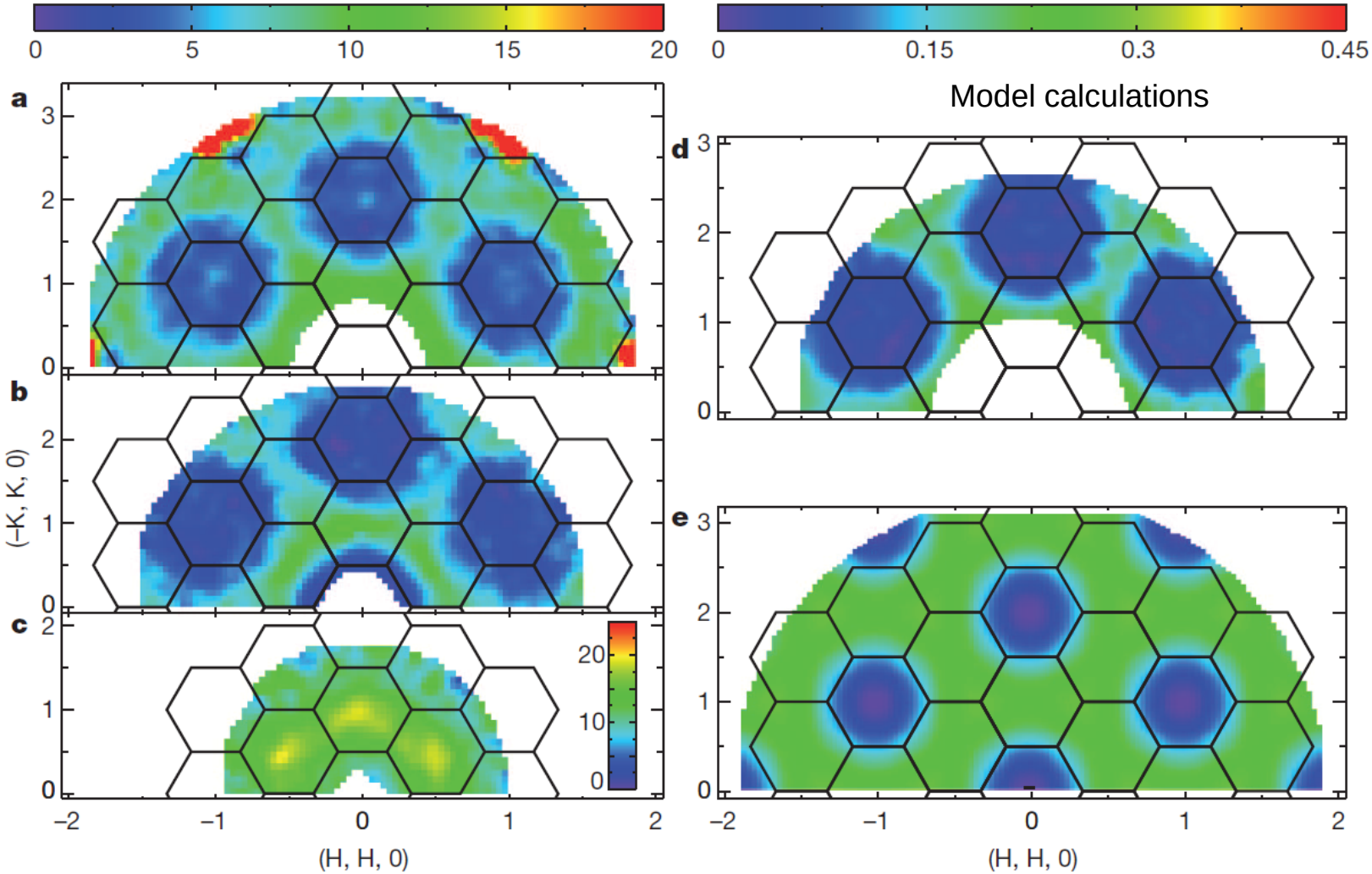
Rodriguez et. al., unpublished

QUANTUM SPIN LIQUID

E = 6 meV

E = 2 meV

E = 0.75 meV

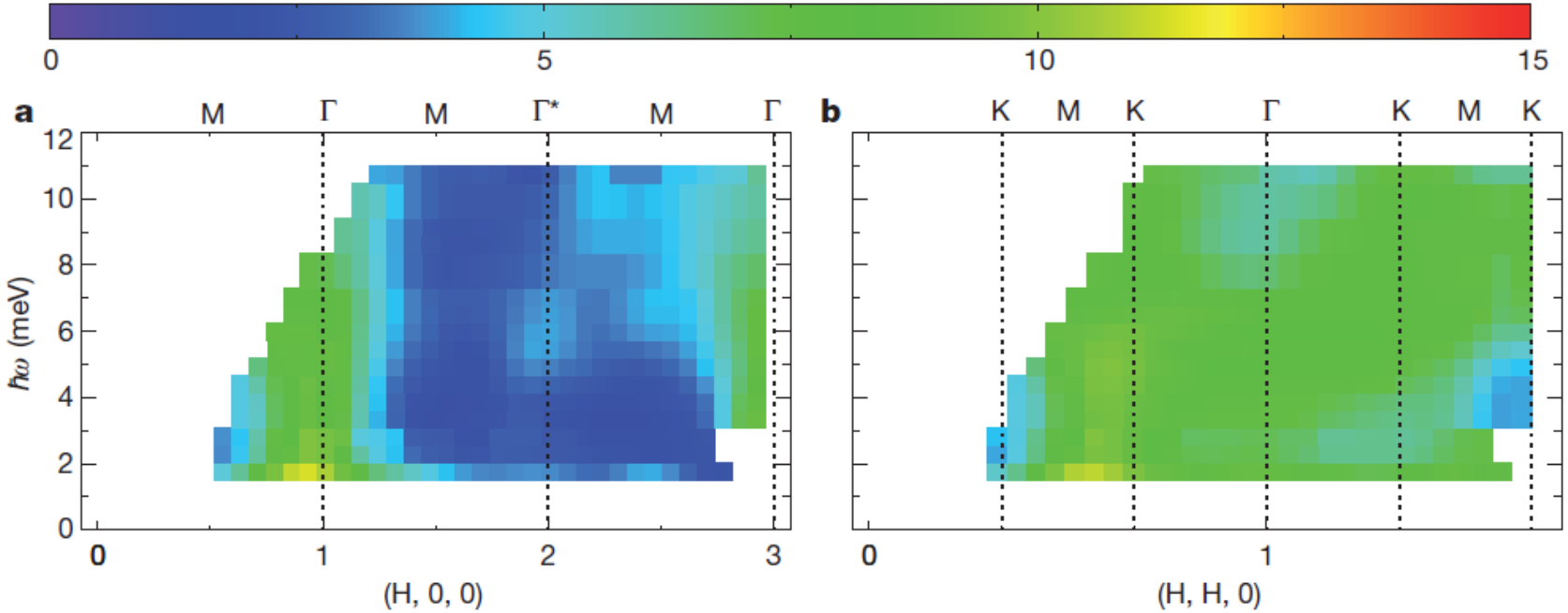


T = 1.6 K

Diffuse: no sharp features that would indicate the presence of long-range magnetic order

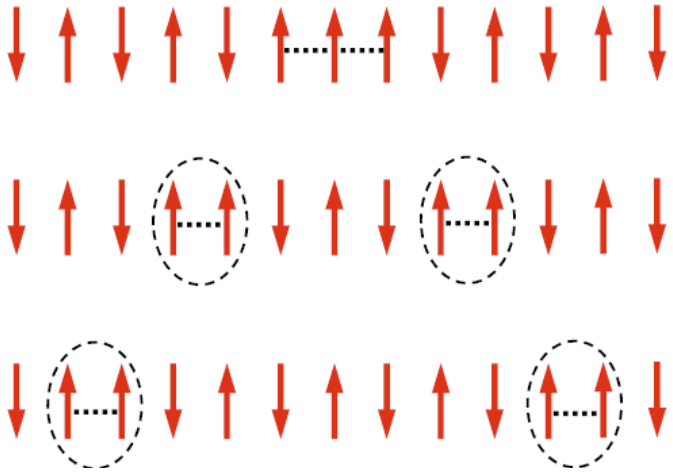
T.-H. Han et. al., Nature **492** 11659 (2012)

QUANTUM SPIN LIQUID



Continuum of spin excitations in 2-D magnet

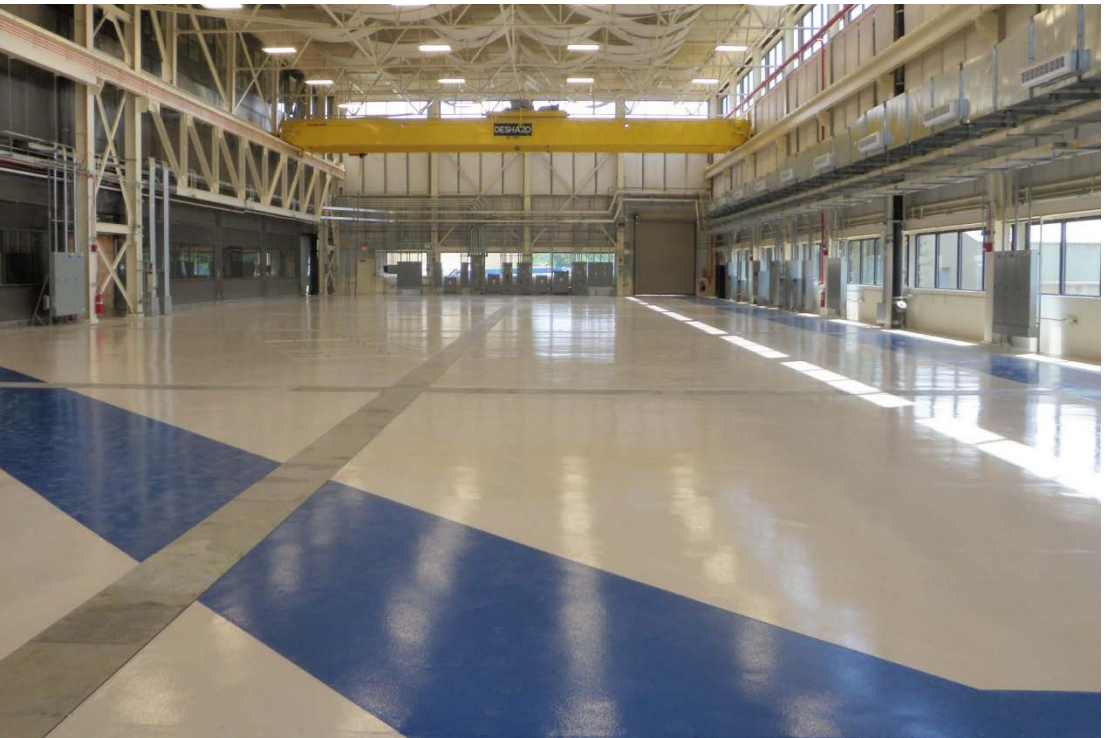
Direct evidence for fractionalized excitations



S=1 excitation breaks up into two S=1/2 spinons

T.-H. Han et. al., Nature **492** 11659 (2012)

Thank You


DESHAZO