Accelerator based facilities as tools for Materials Science

IAEA School on Pulsed Neutron Sources: Enhancing the Capacity for Materials Science

Kurt N Clausen
Condensed Matter Research with Neutrons and Muons
Paul Scherrer Institut
Switzerland

Acknowledgement – thanks to:

The ESS project: D Richter, G Bauer, R McGreevy, CPT, …….
http://neutron.neutron-eu.net/n_documentation/n_reports/n_ess_reports_and_more

SNS – Oak Ridge, USA: T Mason, N Holtkamp, I Anderson, http://www.sns.gov/

J-SNS Japan: M. Arai, … http://jkj.tokai.jaeri.go.jp/

The UK Neutron Strategy Document: www.neutrons.cclrc.ac.uk/Activity/ScienceCase

PSI: W Wagner, S Janssen, Joachim Kohlbrecher, Thomas Gutberlet, E Lehmann, V. Pomjakushin, Christian Rüegg, Henrik Ronnow, R Bercher, H Luetkens plus LNS and LMU
http://www.psi.ch
http://www.psi.ch/forschung/benutzerlabor.shtml

On many slides you will find a text box like this: This signifies that part or all of the information on the slide has been contributed by the named person from the mentioned institution

Name, Institution

The contributions from the above named individuals and reports are gratefully acknowledged.

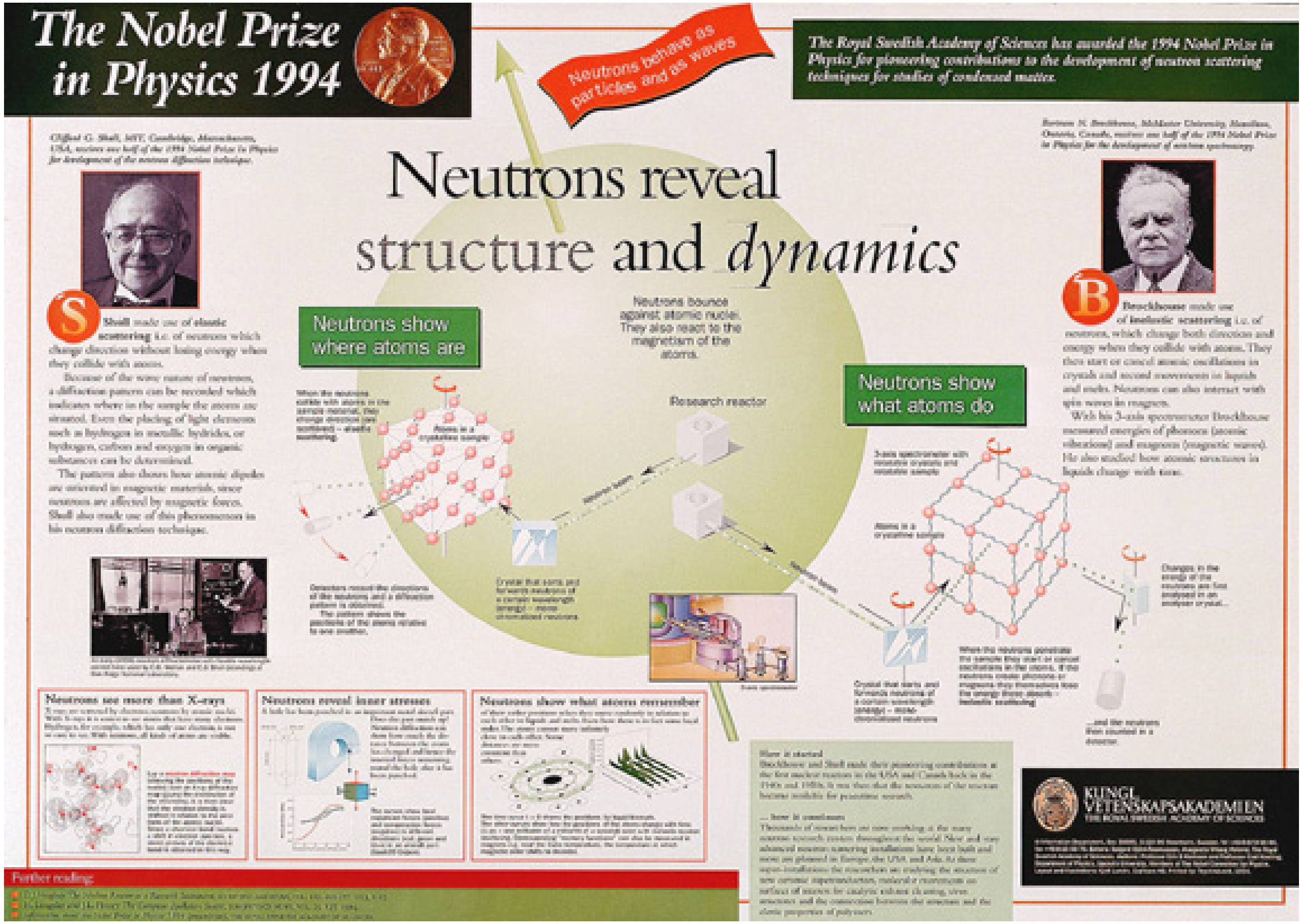
Neutrons and Neutron Sources

1932
The neutron was discovered in by Chadwick in the UK

1936
Coherent neutron diffraction (Bragg scattering by crystal lattice planes) was first demonstrated by two groups in Europe in order to better understand neutrons themselves

> 1945
The possibility of using the scattering of neutrons as a probe of materials developed with the availability of copious quantities of slow neutrons from reactors. Enrico Fermi's group in Chicago used Bragg scattering to measure nuclear cross-sections.

1994
Nobel Prize in Physics – B Brockhouse and C Shull


The Nobel Prize
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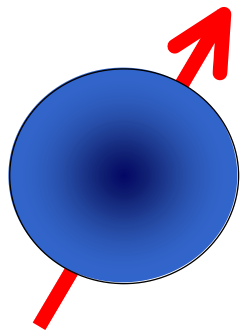
Neutrons behave as particles and as waves
The Royal Swedish Academy of Sciences has awarded the 1994 Nobel Prize in Physics for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter.
Neutrons reveal
structure and dynamics
Neutrons show where atoms are
Neutrons bounce against atomic nuclei. They also react to the magnetism of the atoms.
Research reactor
Neutrons show what atoms do
Neutrons see more than X-rays
Neutrons reveal inner stresses
Neutrons show what atoms remember
Further reading
KUNGL. VETENSKAPSAKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

1994

The neutron..

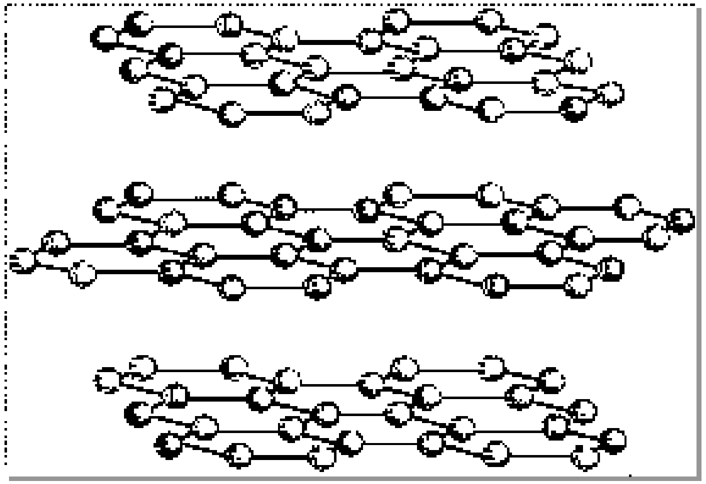
Mass	$1.674928 \cdot 10^{-27}$ kg
Spin	$-\hbar/2$
Magnetic Moment	$-9.6491783 \cdot 10^{-27}$ J/T
Lifetime	885.9 ± 0.9 s
Confinement radius	0.7 fm
Quark structure	udd



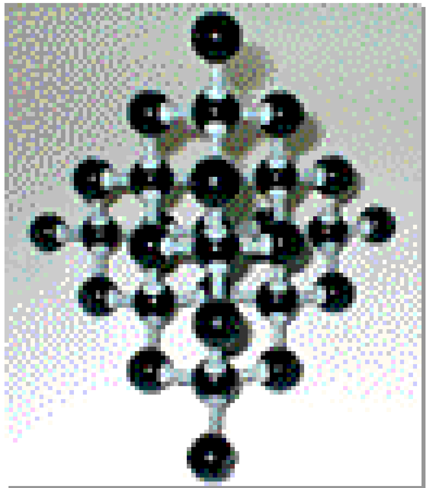
$$n \rightarrow p^+ + e^- + \nu$$

Structure determines properties

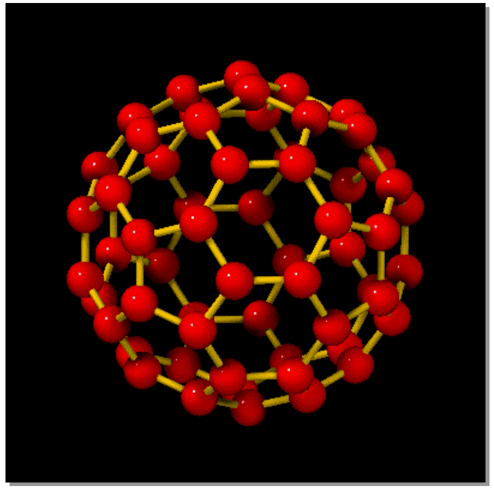
Three forms of carbon – very different materials



Graphite



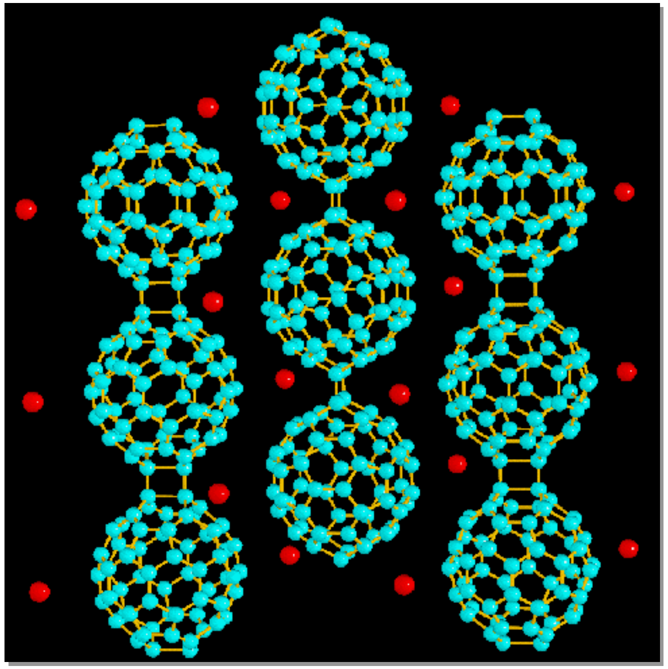
Diamond

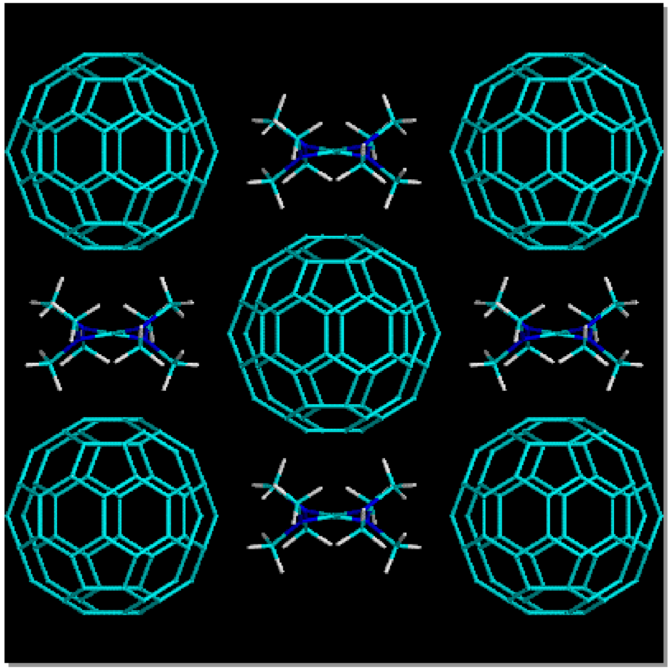


Buckyballs

T Mason, SNS

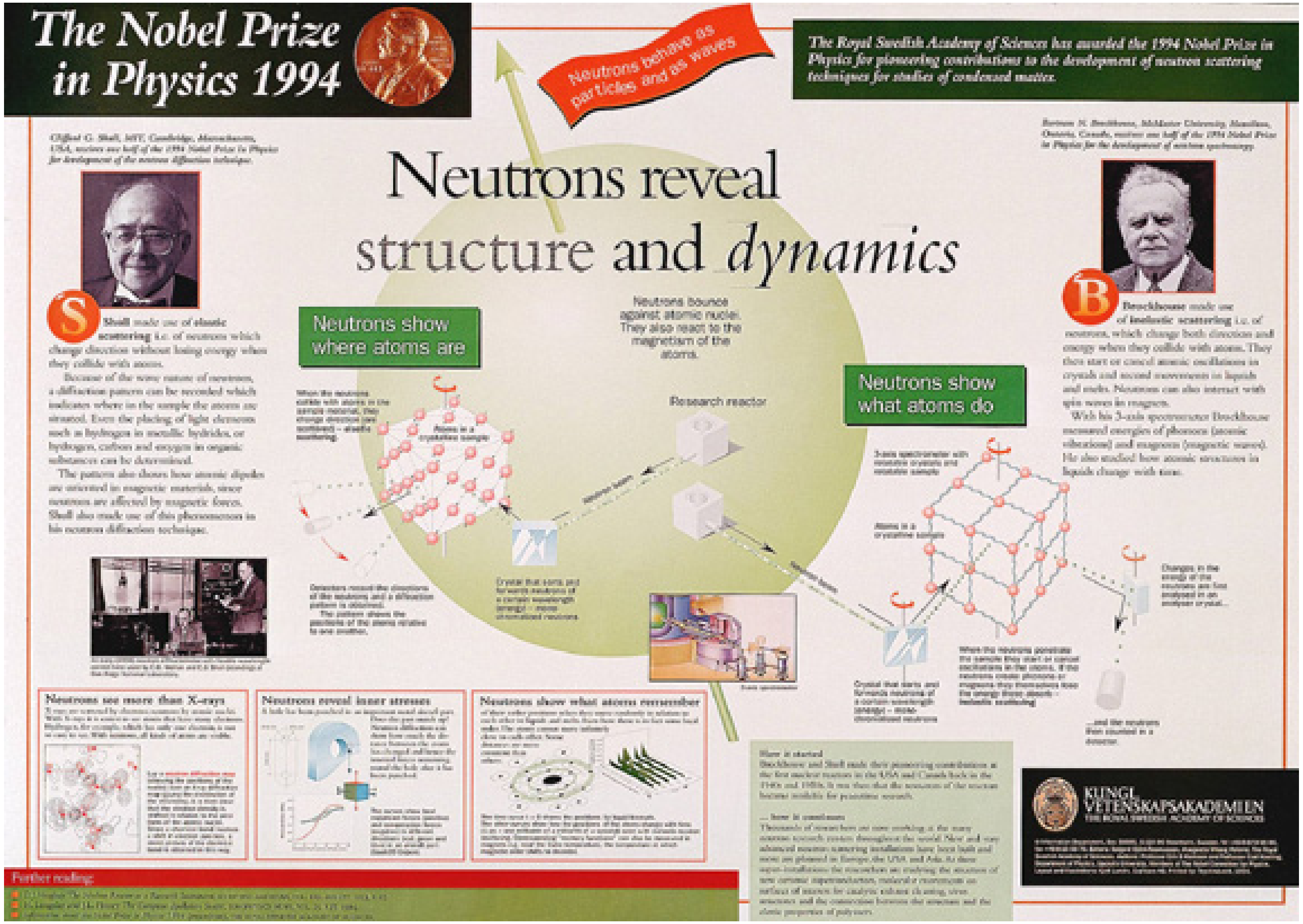
Structure and dynamics determines "function"





Superconductors or organic ferromagnets

T Mason, SNS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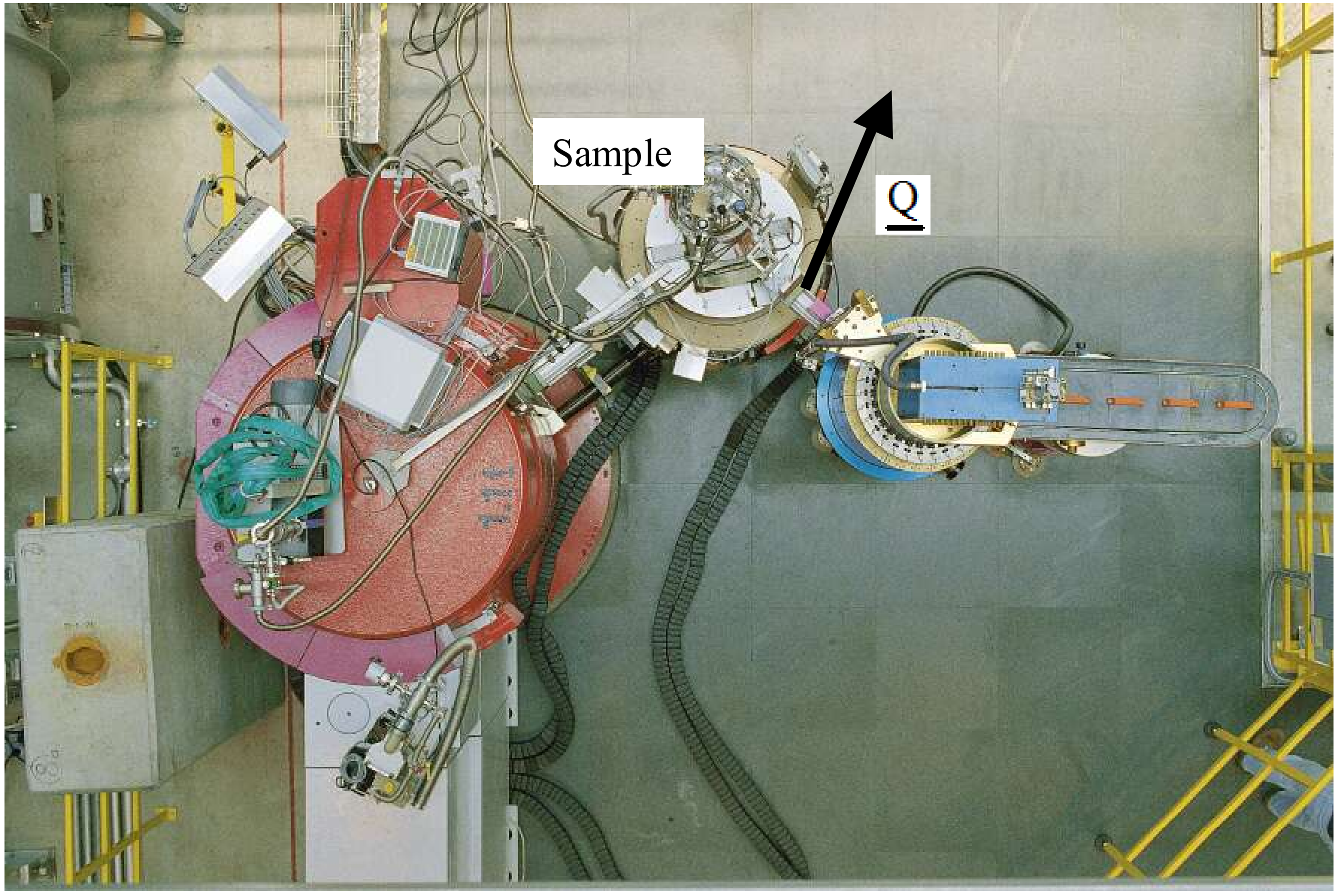
1994

A generic spectrometer

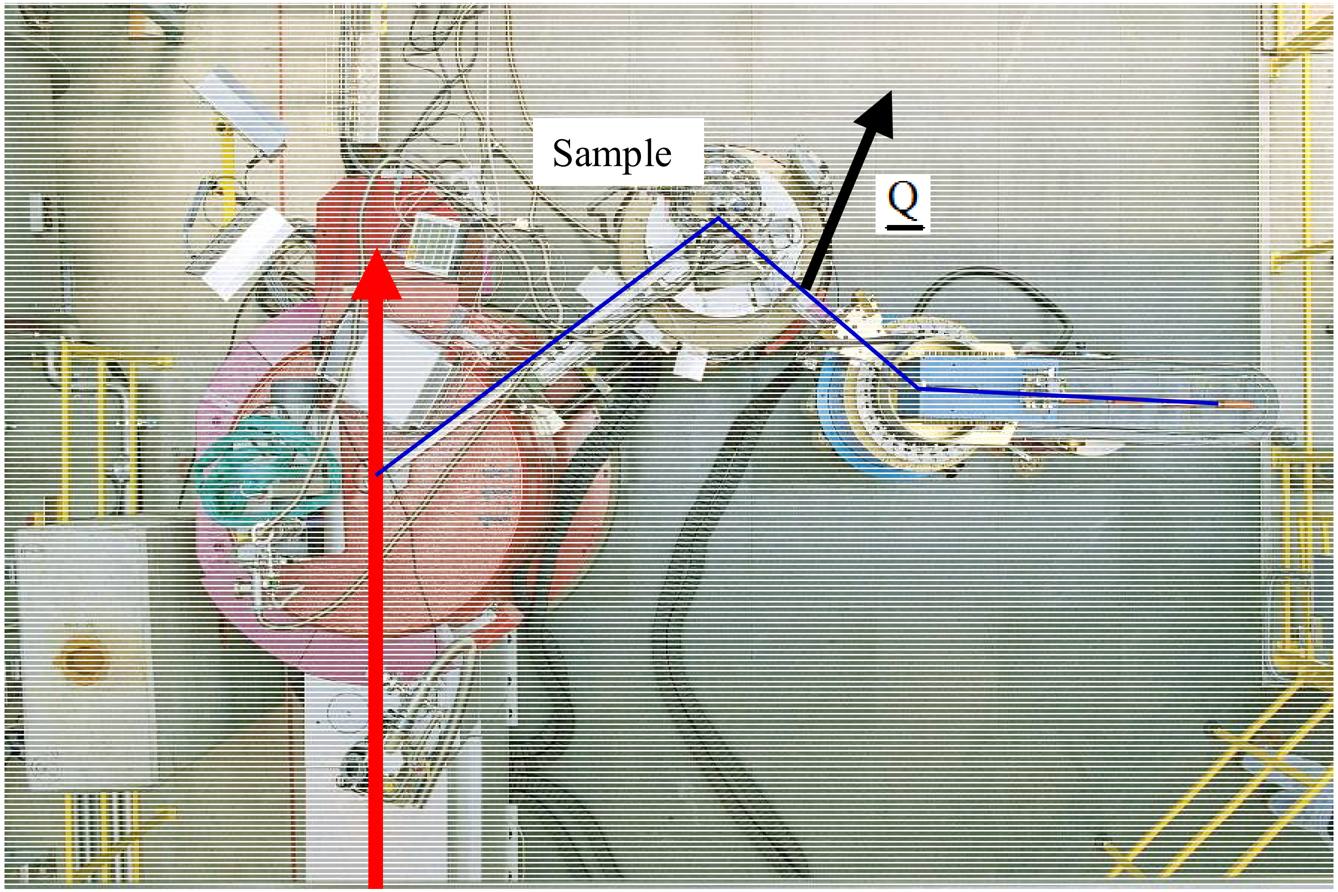


$$|\underline{k}| = \frac{2\cdot\pi}{\lambda}$$

Energy transfer to sample $E = \frac{\hbar^2}{2\cdot m}\left[\underline{k}_i^2 - \underline{k}_f^2\right]$

Wave vector transfer to sample $\underline{Q} = \underline{k}_i - \underline{k}_f$

A generic spectrometer



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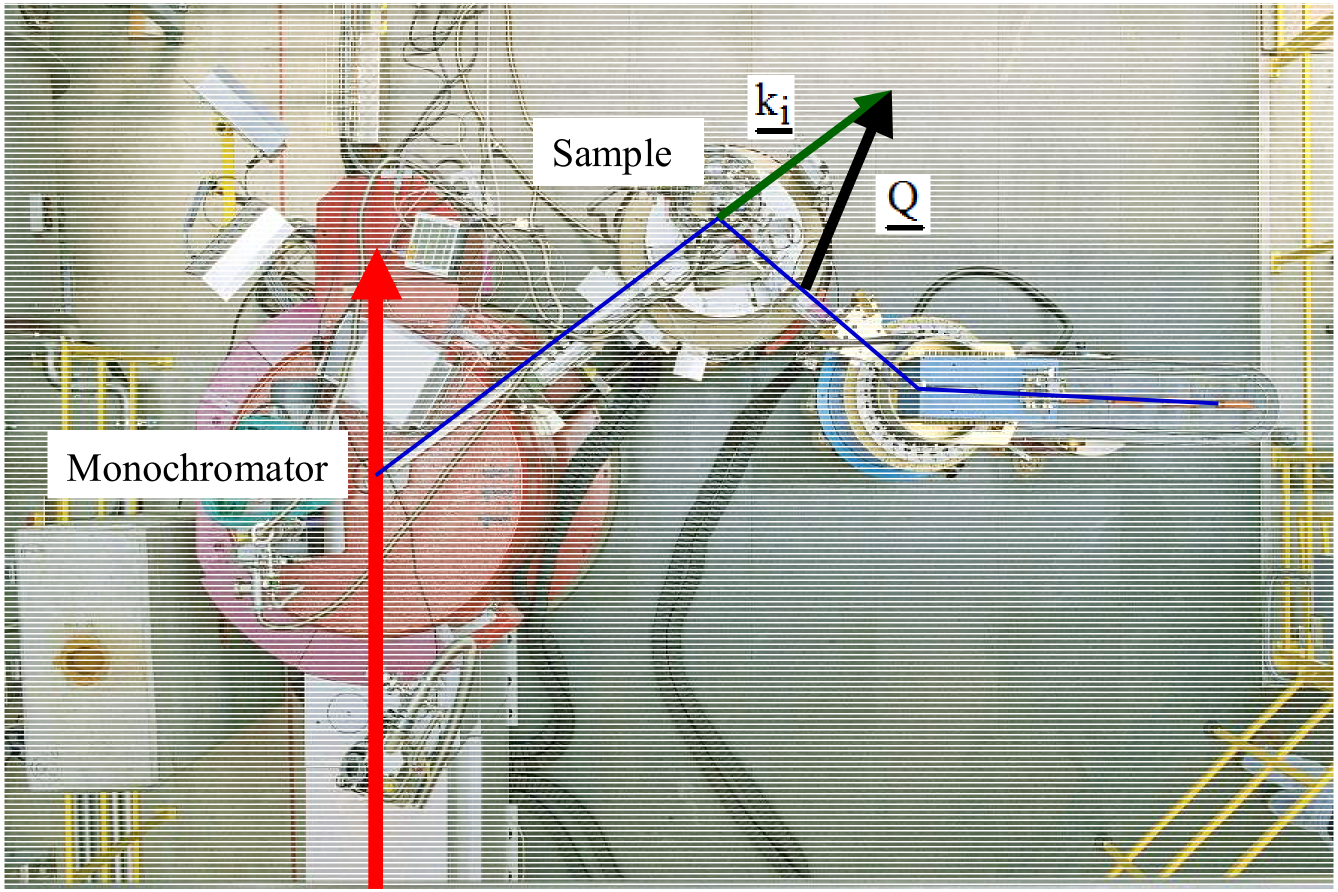

$$|\underline{k}| = \frac{2 \cdot \pi}{\lambda}$$

$$E_i = \frac{\hbar^2 \cdot \underline{k}_i^2}{2 \cdot m}$$

Energy transfer to sample $E = \frac{\hbar^2}{2 \cdot m}\left[\underline{k}_i^2 - \underline{k}_f^2\right]$

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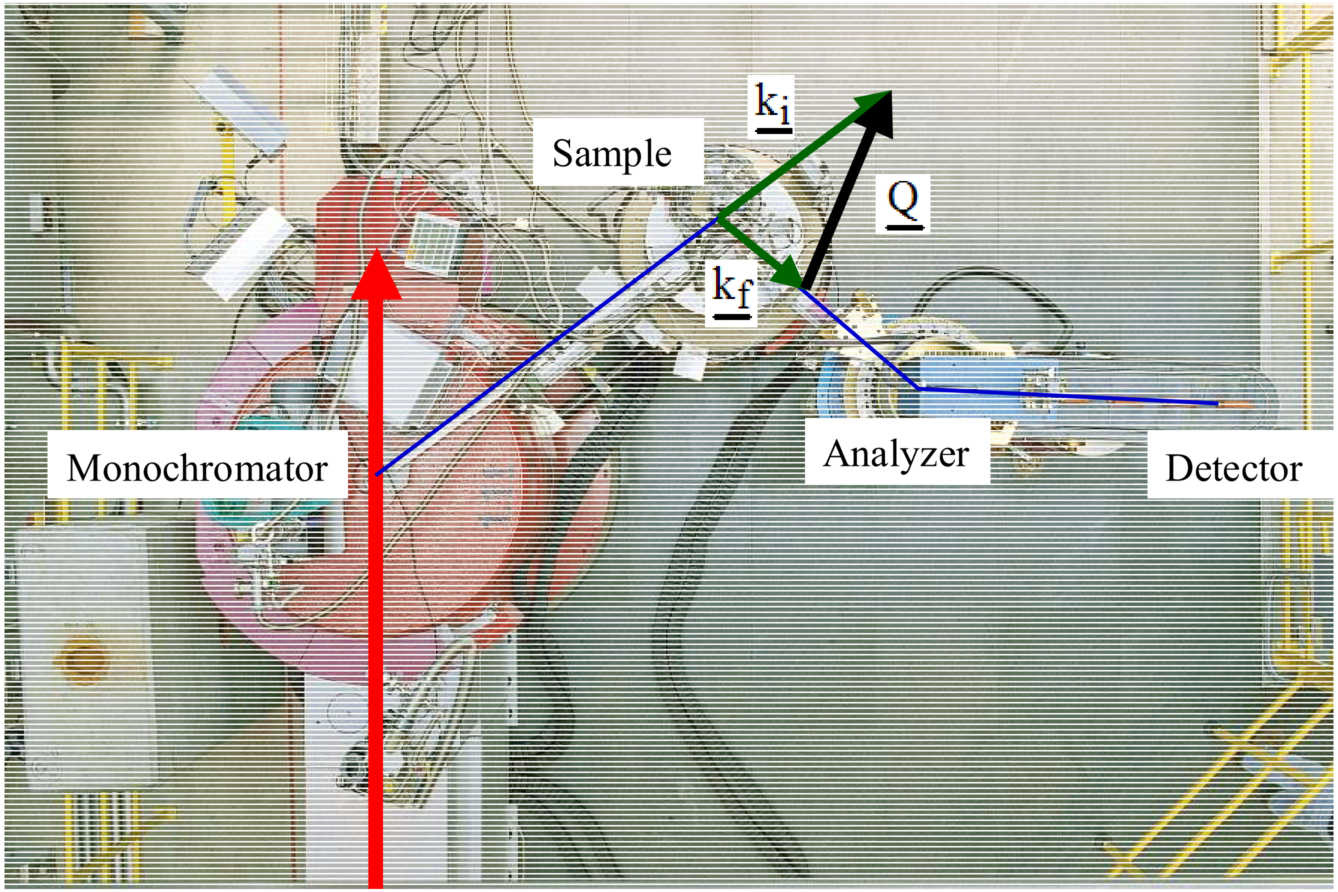

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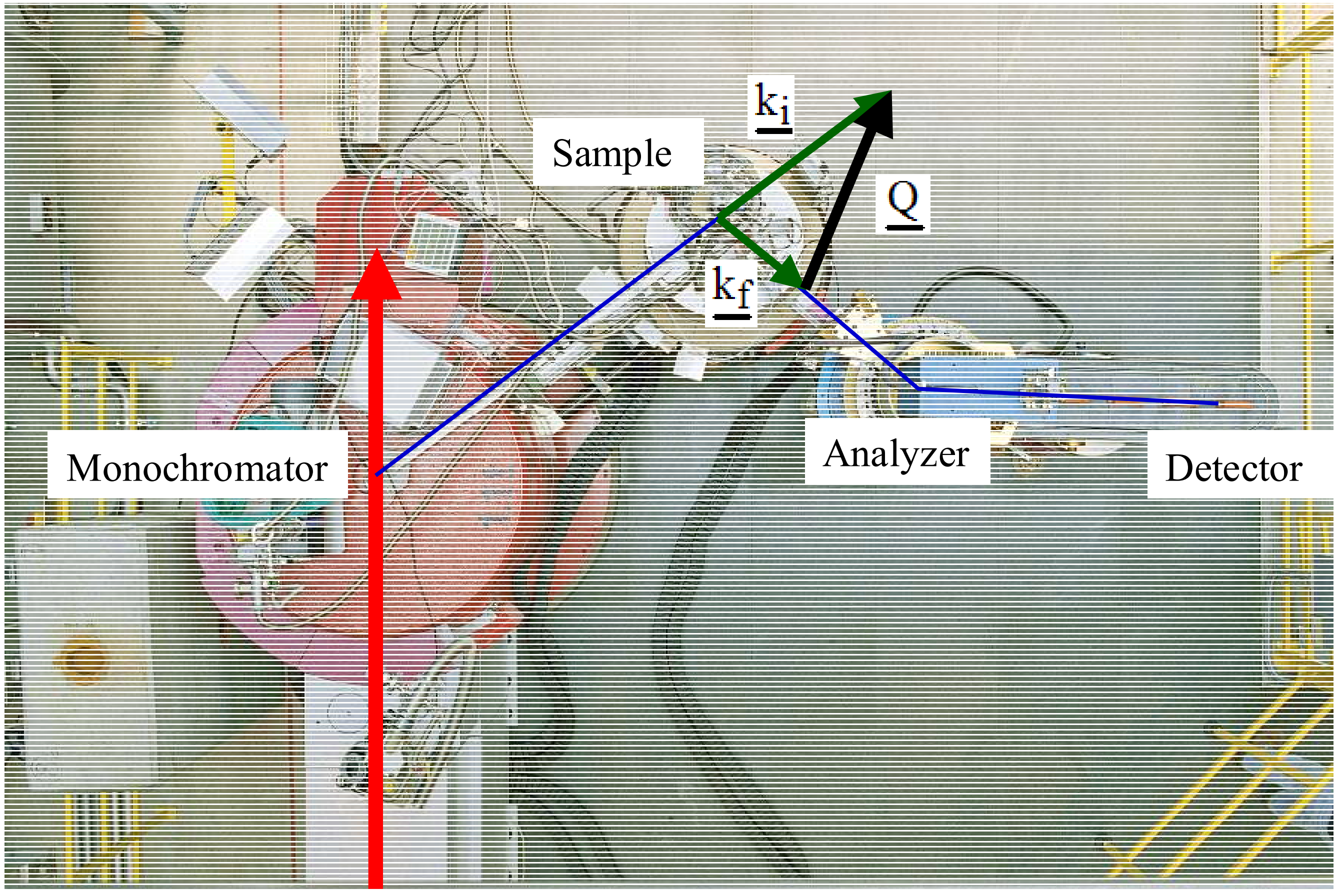

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$$E_f = \frac{\hbar^2 \cdot \underline{k}_f^2}{2 \cdot m}$$

$$E = \hbar\, \omega$$

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Wave vector transfer to sample $\underline{Q} = \underline{k}_i - \underline{k}_f$

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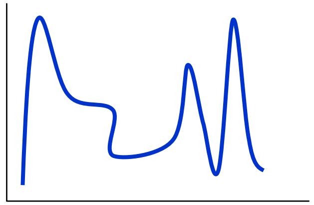
EXAFS **IR absorption**

R McGreevy, ISIS

$\mathbf{k}_2,\ \omega_2$



$I(\mathbf{Q},\omega)$

$\mathbf{Q} = \mathbf{k}_1 - \mathbf{k}_2$

$\omega = \omega_1 - \omega_2$

$G_{AB}(\mathbf{r},t)$

Separation

Transform

$S(\mathbf{Q},\omega) = \Sigma\, S_{AB}(\mathbf{Q},\omega)$

Constant b

Isotopic substitution

Wide $(\mathbf{Q},\omega)$ range

Understanding

Raman scattering **Microscopy** **NMR**

EXAFS

IR absorption

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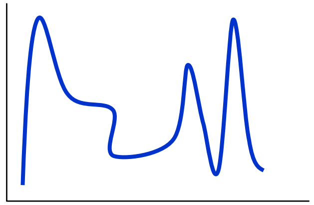

$\mathbf{k}_2,\ \omega_2$

$\mathbf{k}_1,\ \omega_1$

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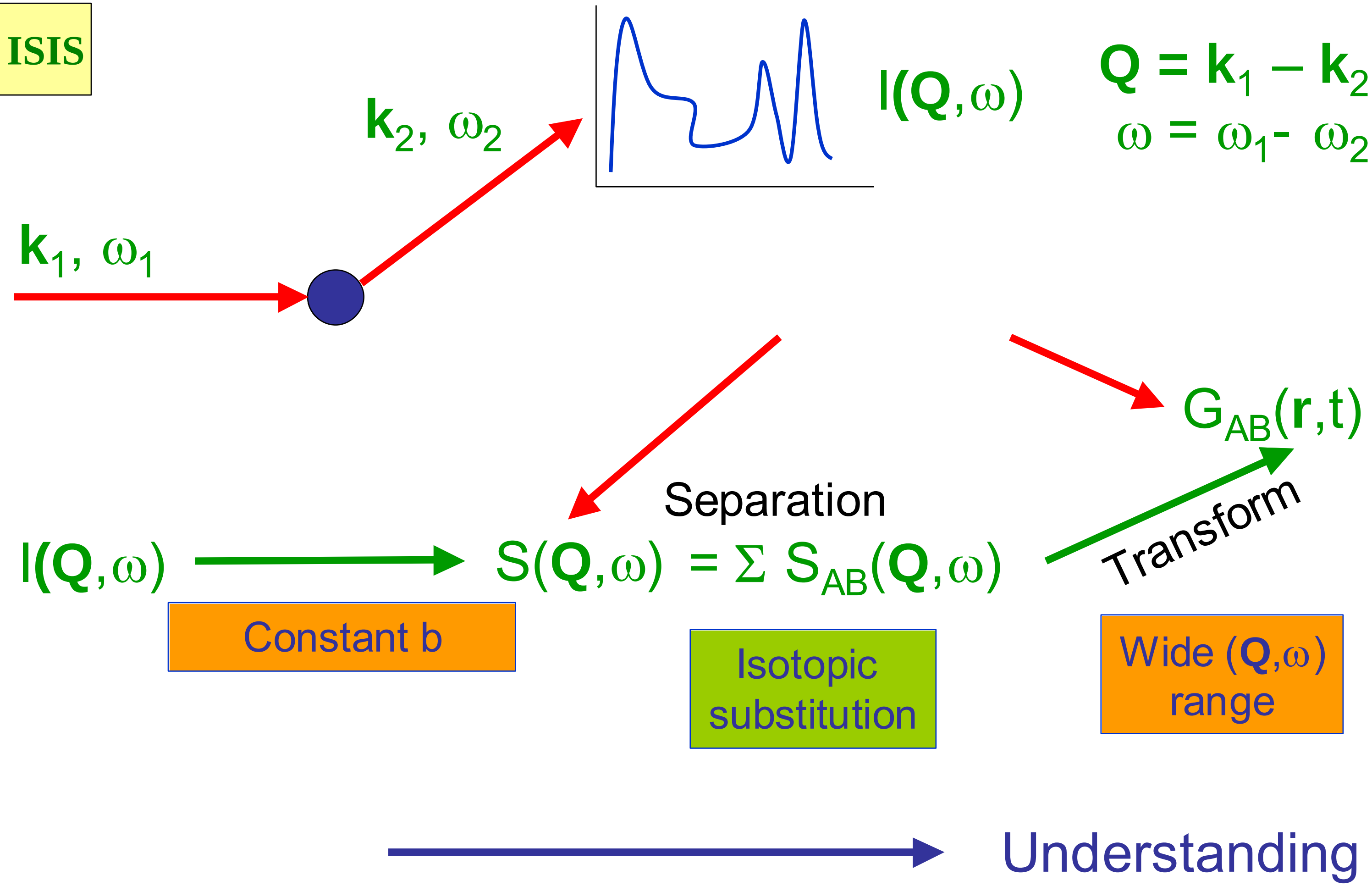

Raman scattering **Microscopy** **NMR**

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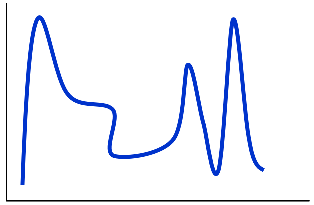

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$\mathbf{k}_1,\ \omega_1$

$G_{AB}(\mathbf{r},t)$

Separation

Transform

$I(\mathbf{Q},\omega) \rightarrow S(\mathbf{Q},\omega) = \Sigma\, S_{AB}(\mathbf{Q},\omega)$

Constant b

Isotopic substitution

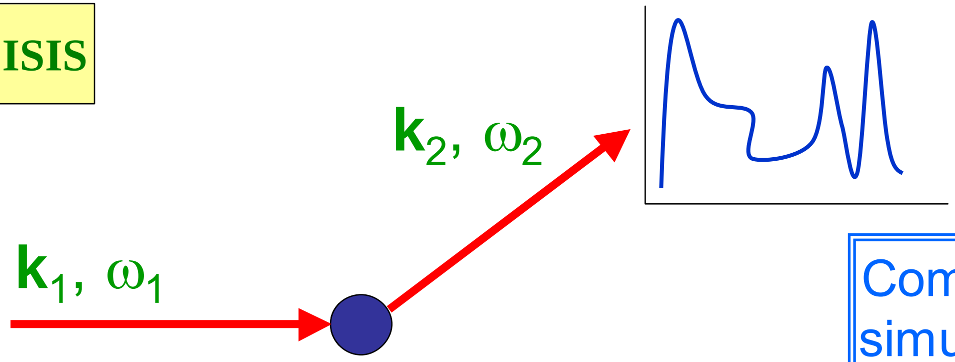
Wide $(\mathbf{Q},\omega)$ range

Measurement → Understanding

Raman scattering **Microscopy** **NMR**

EXAFS **IR absorption**

R McGreevy, ISIS



$I(\mathbf{Q},\omega)$

$\mathbf{Q} = \mathbf{k}_1 - \mathbf{k}_2$

$\omega = \omega_1 - \omega_2$

Computer simulation and modelling → $G_{AB}(\mathbf{r},t)$

$I(\mathbf{Q},\omega)$ → $S(\mathbf{Q},\omega) = \Sigma\, S_{AB}(\mathbf{Q},\omega)$ — Separation — Transform → $G_{AB}(\mathbf{r},t)$

Constant b

Isotopic substitution

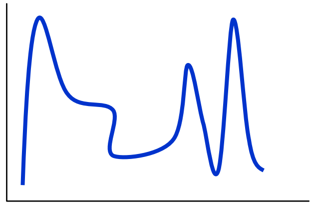
Wide $(\mathbf{Q},\omega)$ range

Measurement → Understanding

Raman scattering **Microscopy** **NMR**

R McGreevy, ISIS

$\mathbf{k}_2, \omega_2$



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$\mathbf{k}_1, \omega_1$

Computer simulation and modelling

$G_{AB}(\mathbf{r},t)$

Separation

Corrections

Transform

$I(\mathbf{Q},\omega)$ → $S(\mathbf{Q},\omega) = \Sigma\, S_{AB}(\mathbf{Q},\omega)$

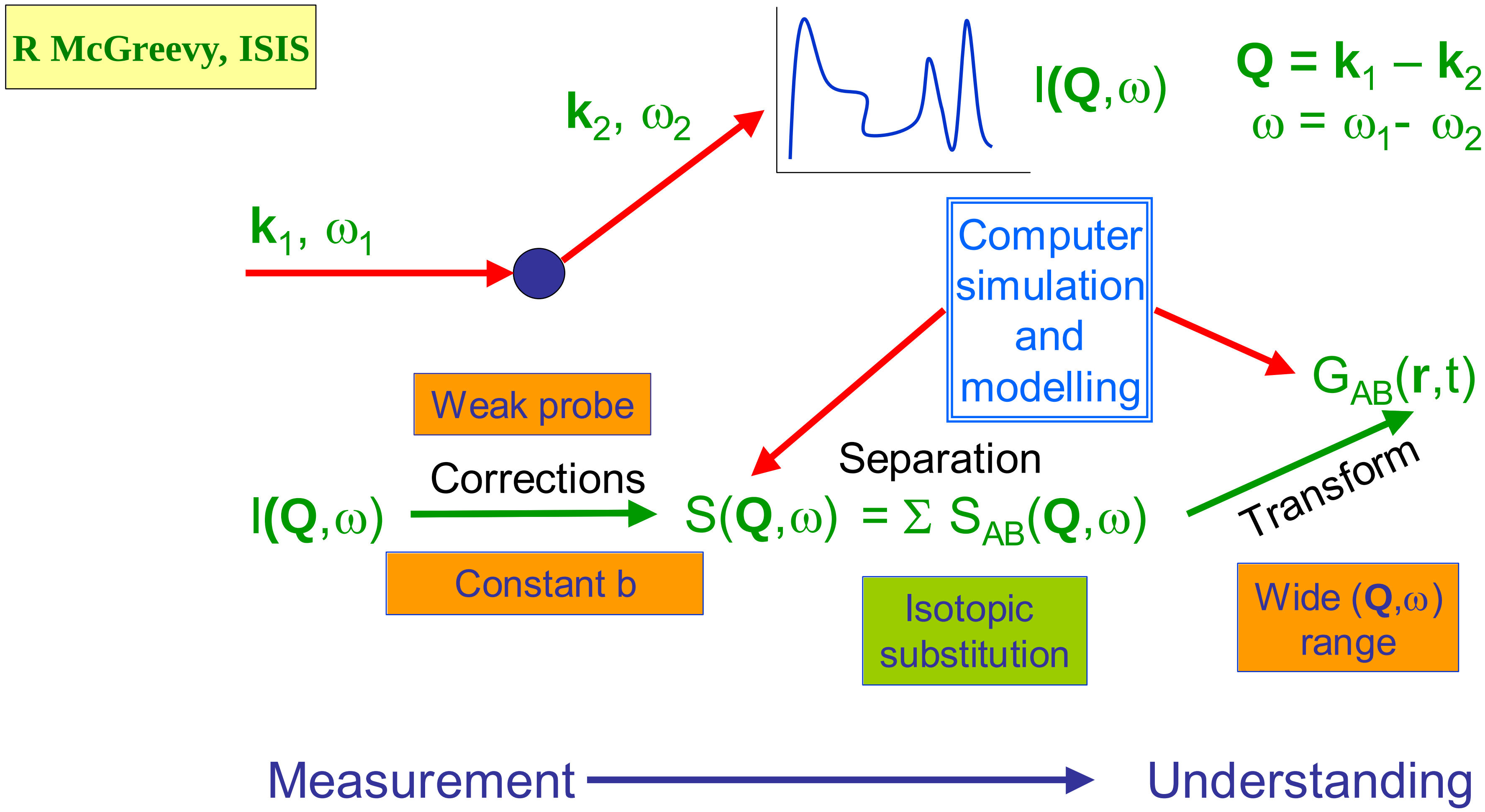
Constant b

Isotopic substitution

Wide $(\mathbf{Q},\omega)$ range

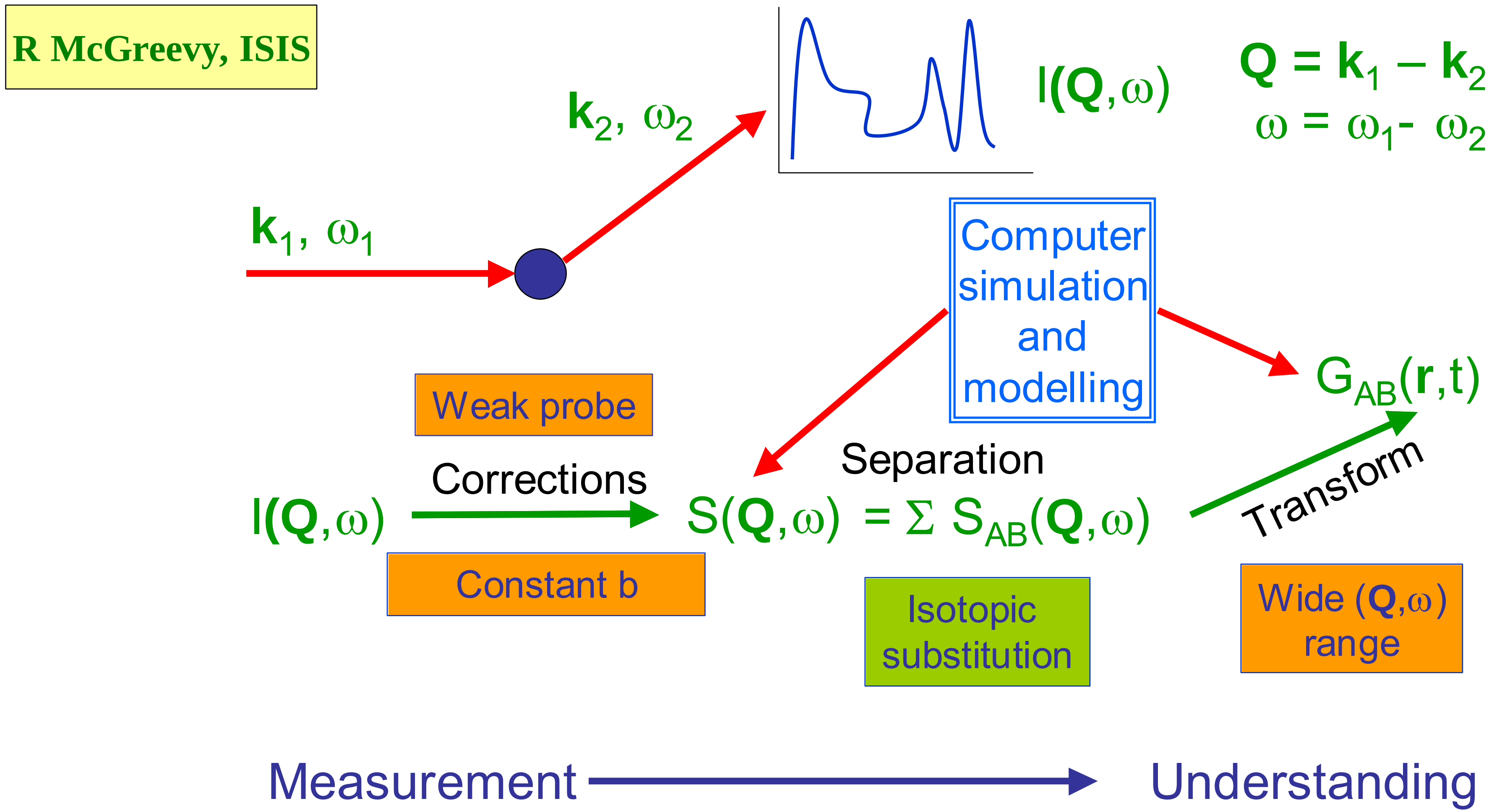
Measurement → Understanding

EXAFS *IR absorption*

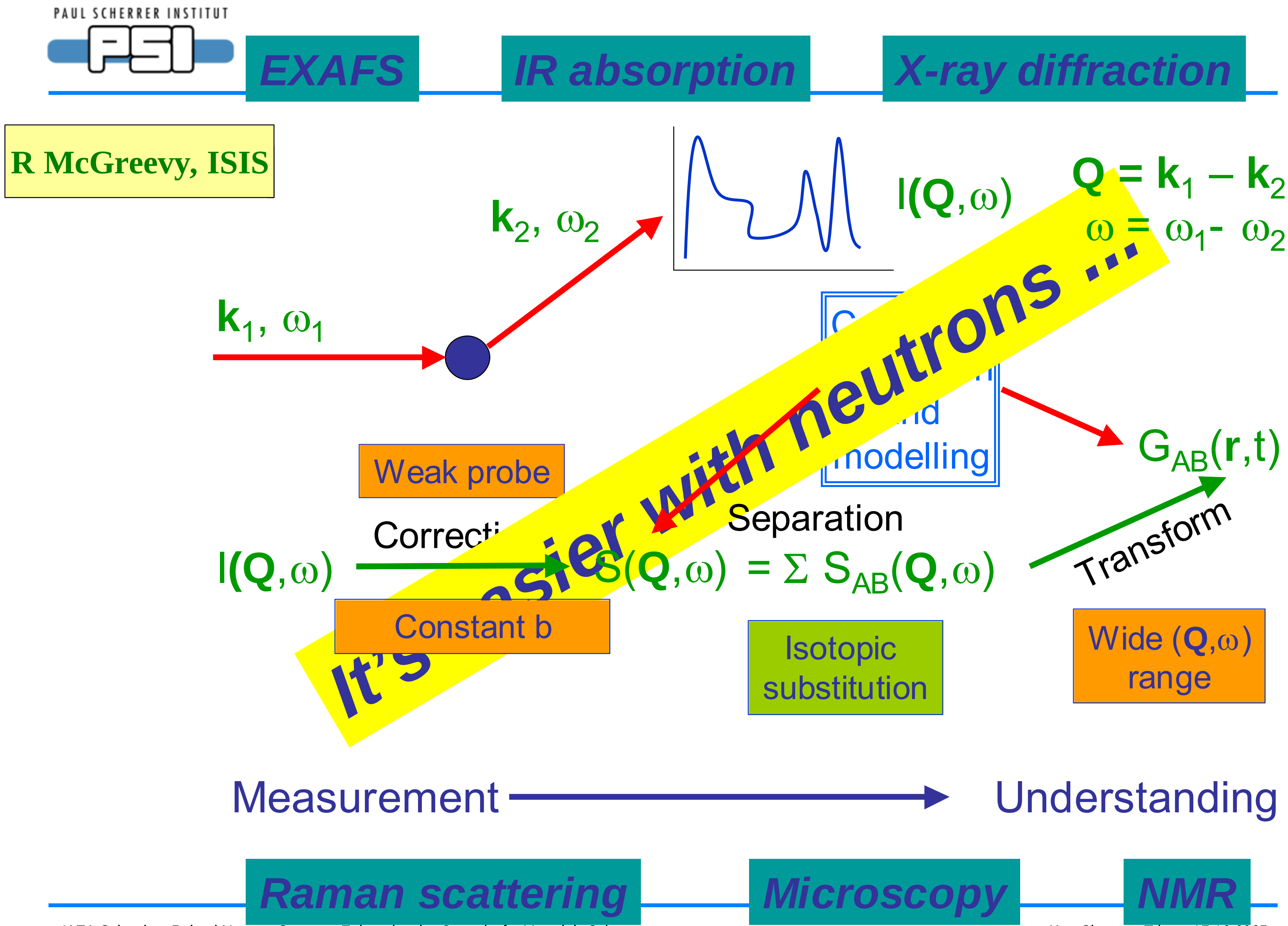


Raman scattering *Microscopy* *NMR*

EXAFS ***IR absorption*** ***X-ray diffraction***



Raman scattering ***Microscopy*** ***NMR***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PSI
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IR absorption
X-ray diffraction
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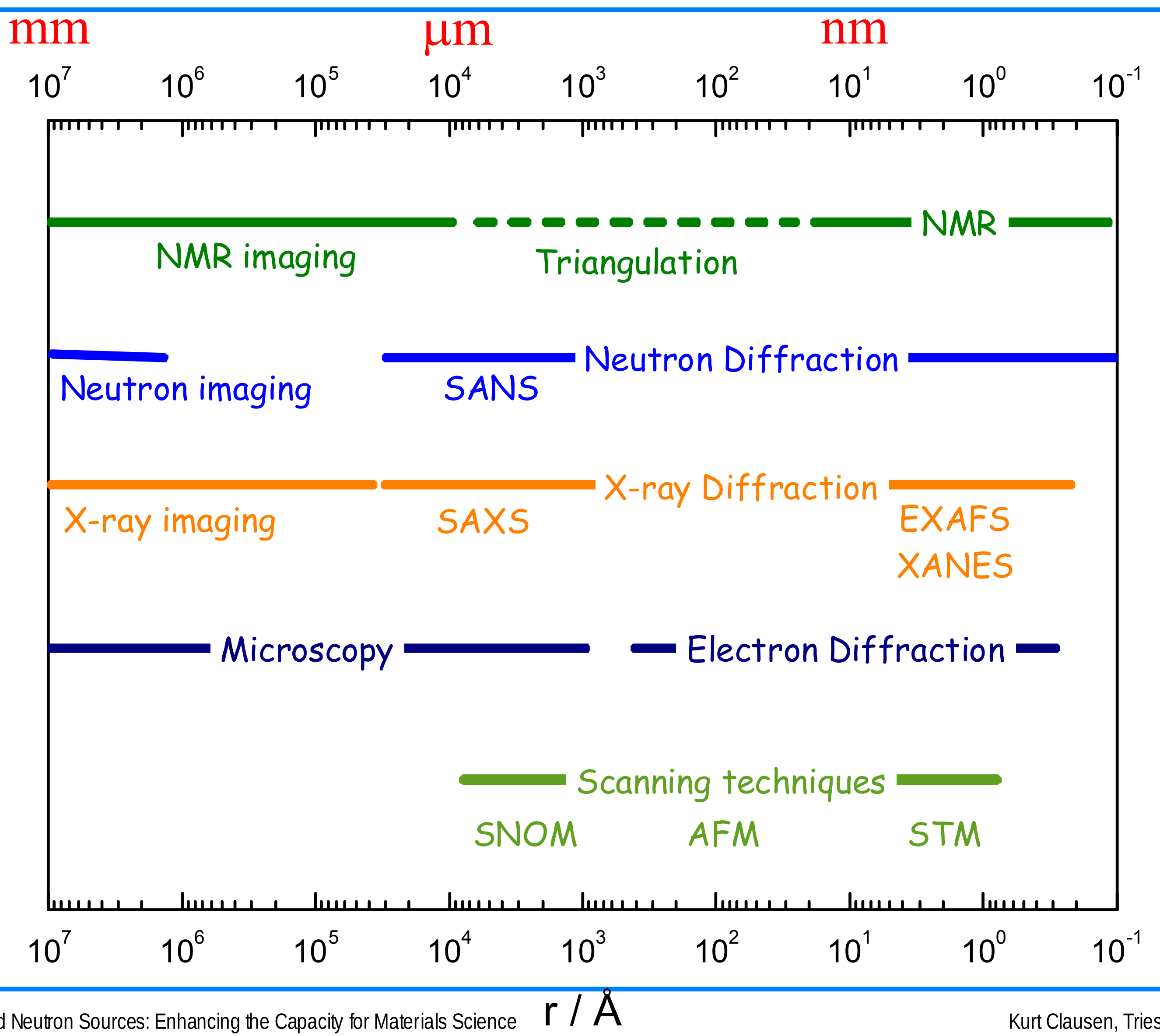
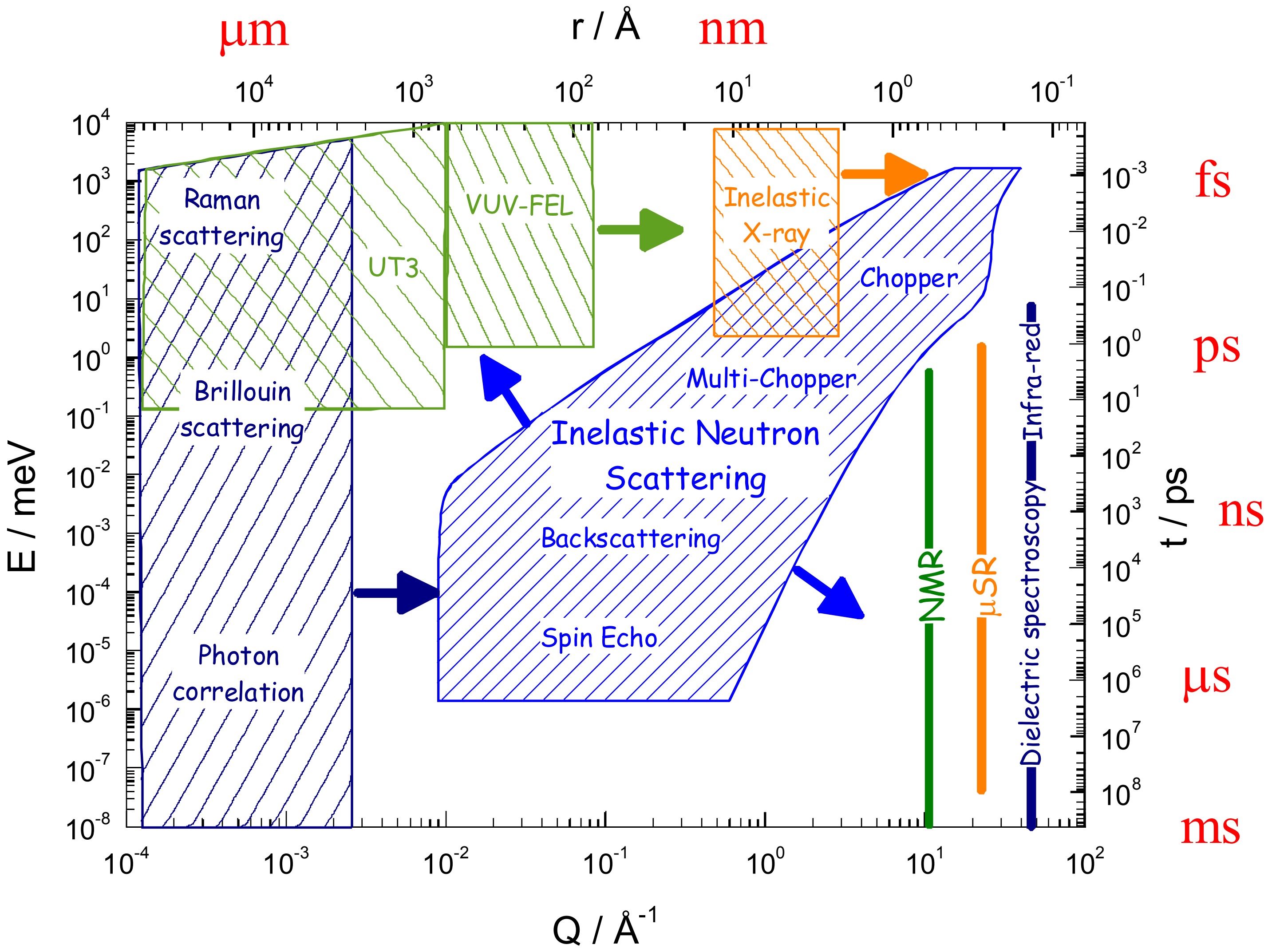
k2, ω2
k1, ω1
I(Q,ω)
Q = k1 – k2
ω = ω1- ω2
modelling
GAB(r,t)
Weak probe
Correcti
Separation
I(Q,ω)
S(Q,ω) = Σ SAB(Q,ω)
Transform
Constant b
Isotopic substitution
Wide (Q,ω) range
It's
sier with neutrons ...
Measurement
Understanding
Raman scattering
Microscopy
NMR

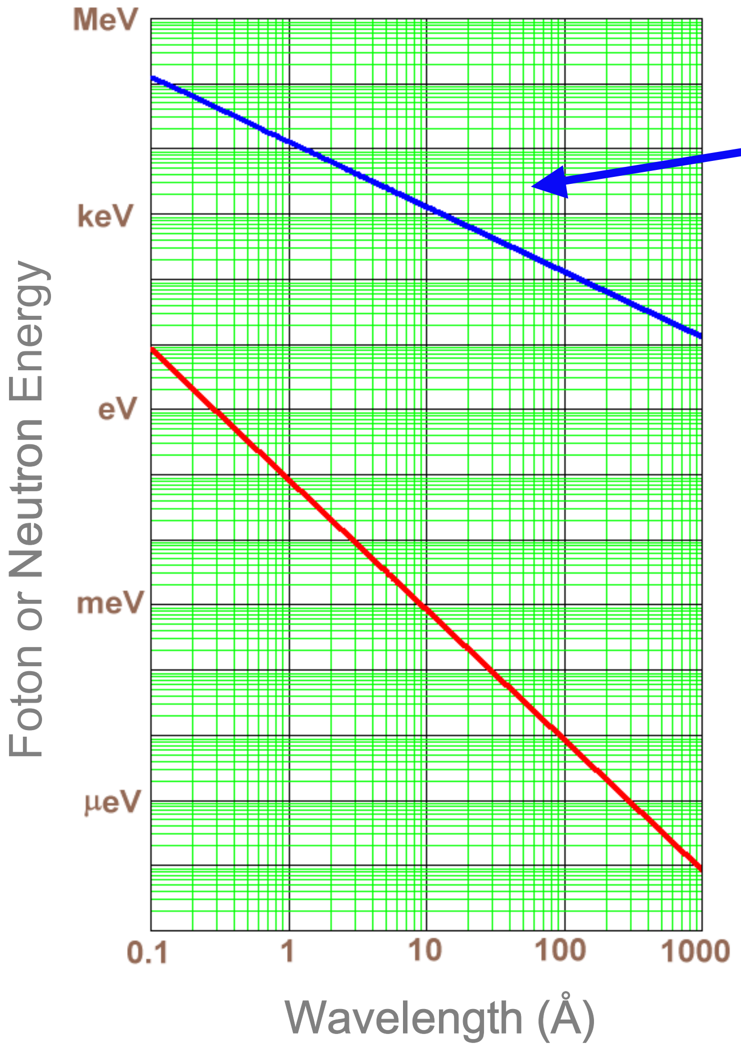
Imaging, Microscopy, Diffraction → *Structure*



Dynamics


µm
r / Å
nm
10^4 10^3 10^2 10^1 10^0 10^{-1}
E / meV
Q / $Å^{-1}$
t / ps
fs
ps
ns
µs
ms
Raman scattering
UT3
VUV-FEL
Inelastic X-ray
Chopper
Brillouin scattering
Multi-Chopper
Inelastic Neutron Scattering
Backscattering
Spin Echo
Photon correlation
NMR
µSR
Dielectric spectroscopy
Infra-red

Neutrons for Condensed Matter Science E < 1 eV



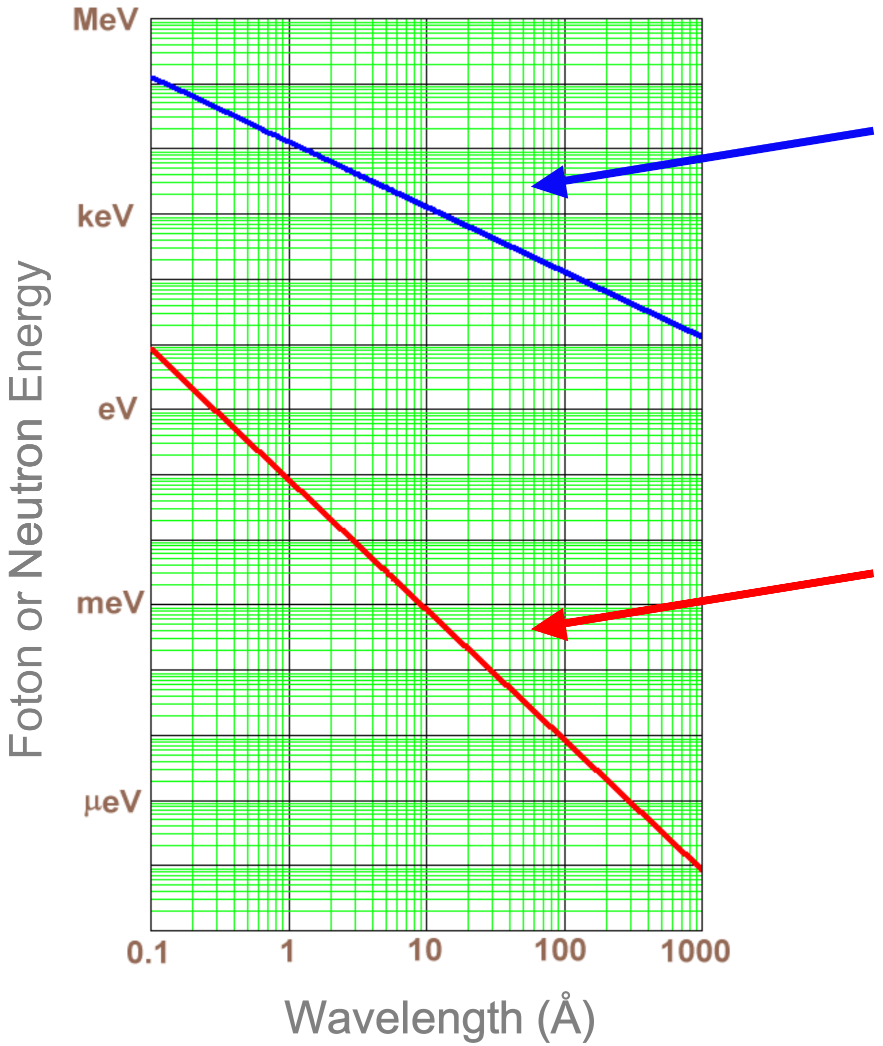
Fotons:

$$E = \frac{h \cdot c}{\lambda}$$

$(h \cdot \nu)$

$$E = \hbar\, \omega$$

Neutrons for Condensed Matter Science E < 1 eV



Fotons:

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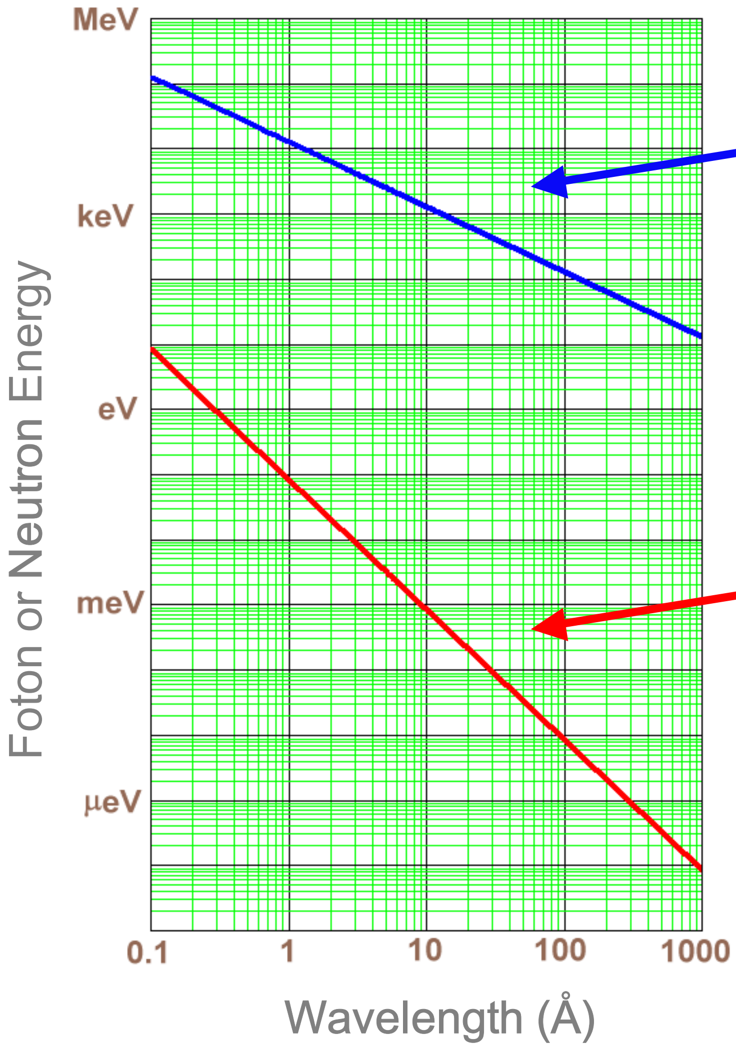
Neutrons:

m = 1.67 10^{-27} kg ~ m_{proton}

Spin = ½

Charge = 0

Neutrons for Condensed Matter Science E < 1 eV



Fotons:

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Neutrons:

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Spin = ½

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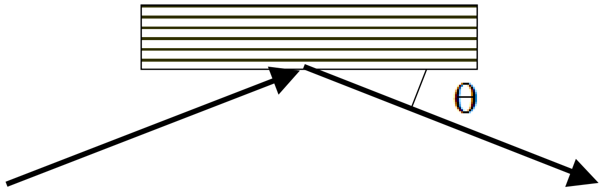
$$E = \frac{h^2}{2 \cdot m \cdot \lambda^2} \quad \left(\tfrac{1}{2} \cdot m \cdot v^2\right)$$

Determination of k_i and k_f

Using crystals



$$\lambda = 2 \cdot d \cdot \sin(\theta)$$

$$|\underline{k}| = \frac{2 \cdot \pi}{\lambda}$$

$$\lambda = \frac{h}{m \cdot L} \cdot t$$

$$|\underline{k}| = \frac{2 \cdot \pi}{\lambda}$$

Determination of k_i and k_f

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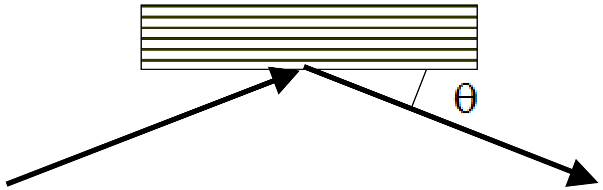

$$\lambda = 2 \cdot d \cdot \sin(\theta)$$

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Using time of flight

$$\lambda = \frac{h}{m \cdot L} \cdot t$$

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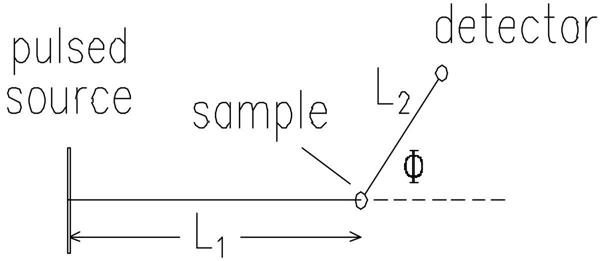

Neutron scattering is an intensity limited technique

The same number of fotons/neutrons will be emitted from:

- 1 W *light bulp* of 2 eV visible light
- 6 kW conventional *X-ray source* of 12 keV radiation
- 100 MW *nuclear reactor* (200 MeV per neutron)

The source size for the reactor is of dimensions m^3 for the others mm^3.

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Why bother about “Candles” when we have synchrotron X-ray sources and soon free electron lasers?

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A large number of presentations in the following two weeks will demonstrate that neutrons in many areas are complementary, in some areas competitive and in others unique.

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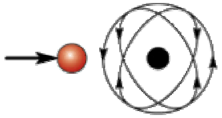
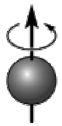
Neutrons : weak source strength – powerful tool for science!

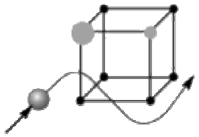
Uniqueness of Neutrons



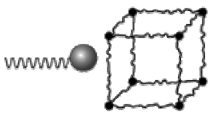
1. Neutrons see the Nuclei



2. Neutrons see Elementary Magnets

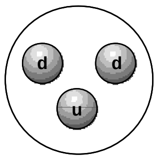


3. Neutrons see light Atoms next to Heavy Ones



4. Neutrons measure the Velocity of Atoms

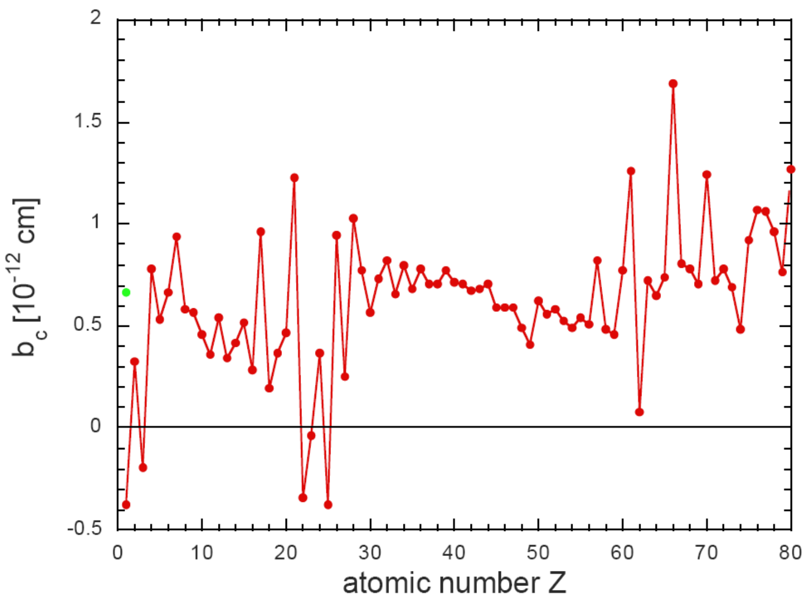
5. Neutrons penetrate deep into Matter



6. Neutrons are Elementary Particles

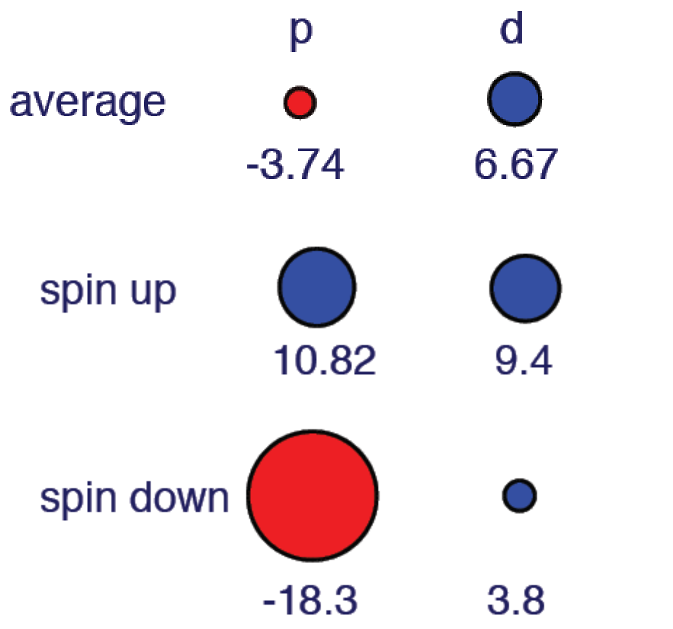
Neutron Scattering Length [fm]

	p	d	C	N	O	P	S
average	-3.74	6.67	6.65	9.36	5.81	5.13	2.85

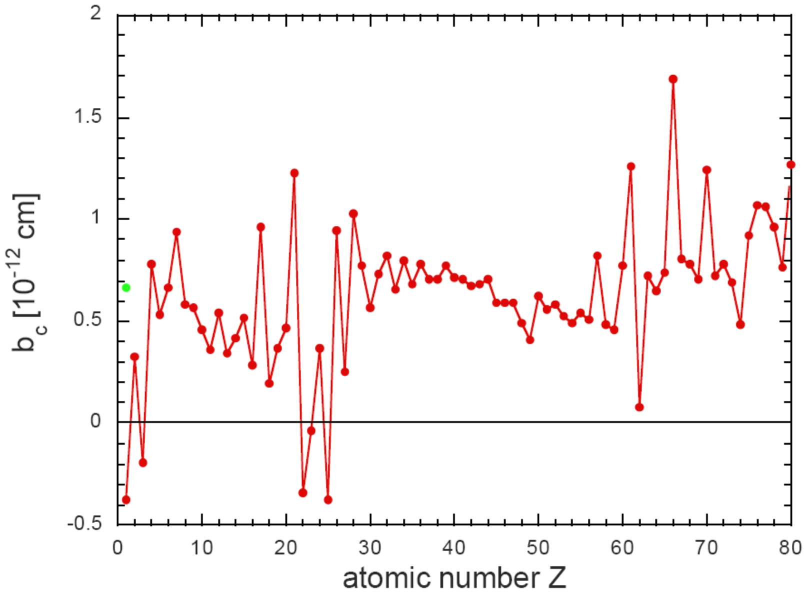


1 fm = 0.1×10^{-12} cm

Neutron Scattering Length [fm]



Spin-dependent scattering lengths

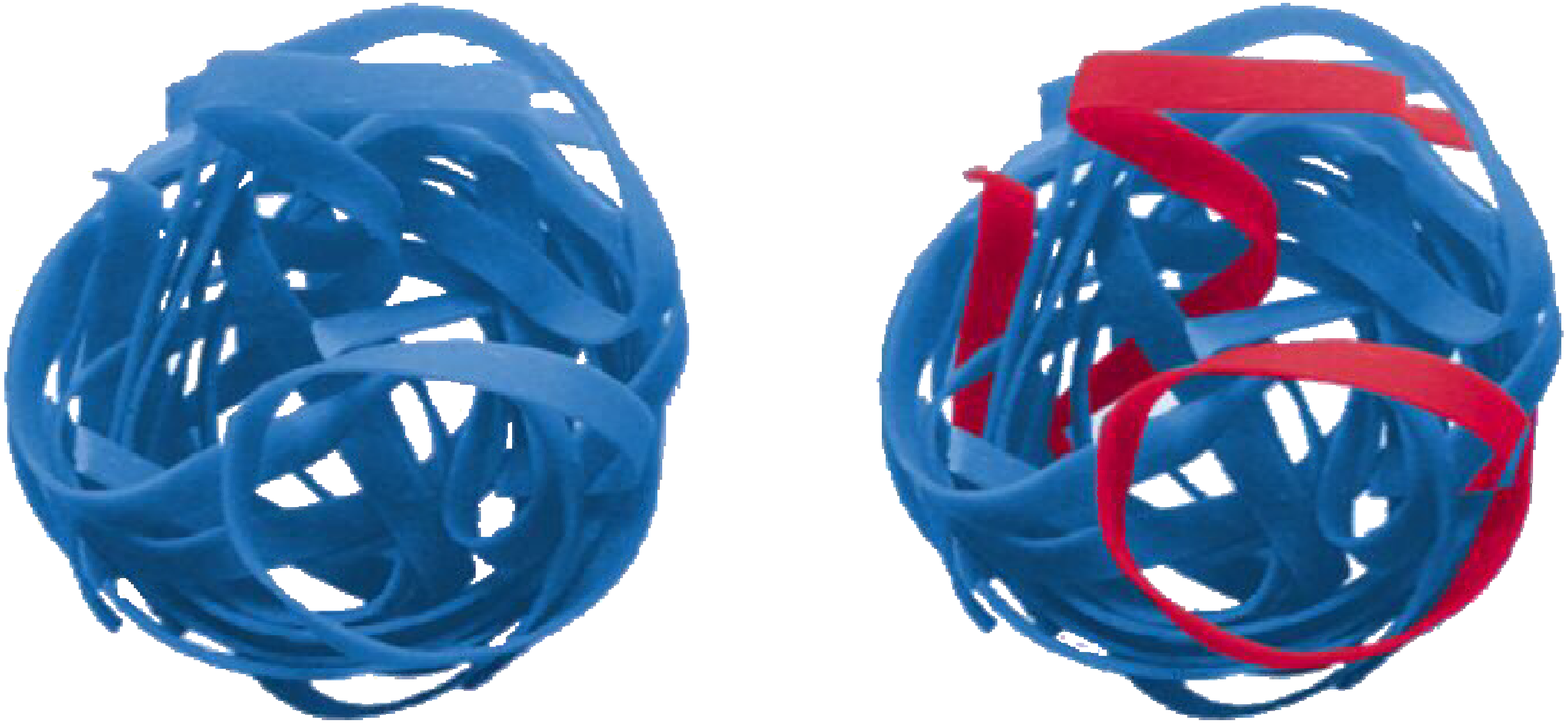


1 fm = 0.1×10^{-12} cm

Contrast Variation

J Kohlbrecher PSI

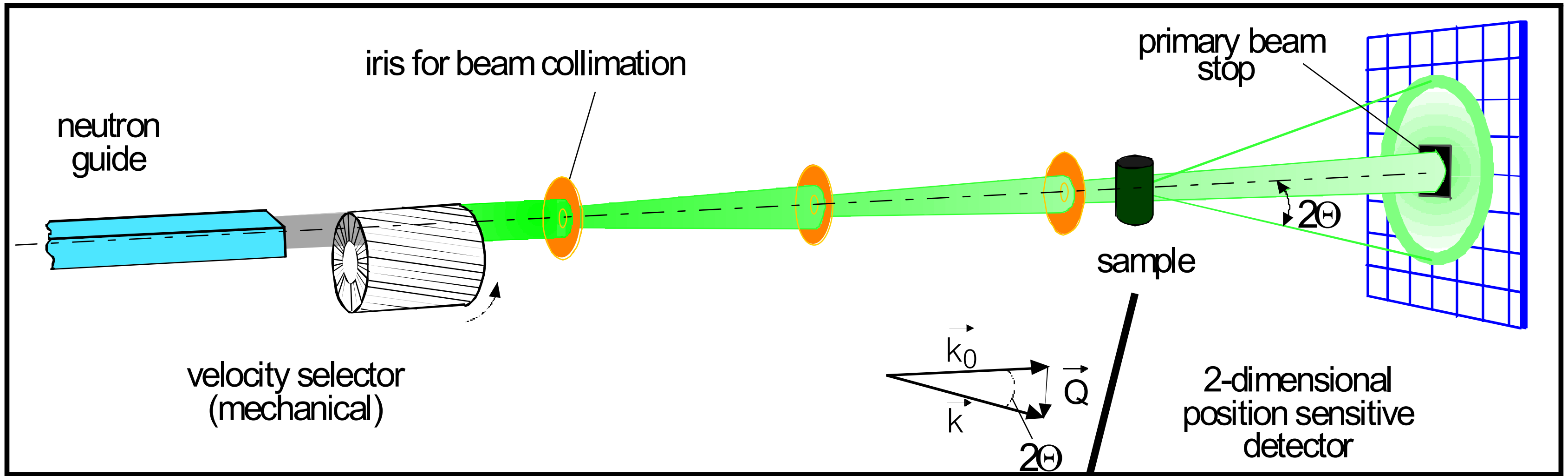
Neutrons see the Nuclei



Isotopic contrasting.

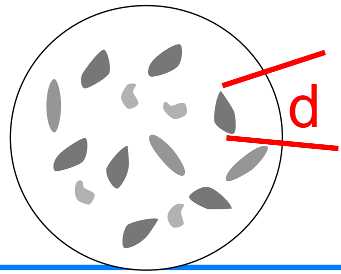
Small Angle Neutron Scattering

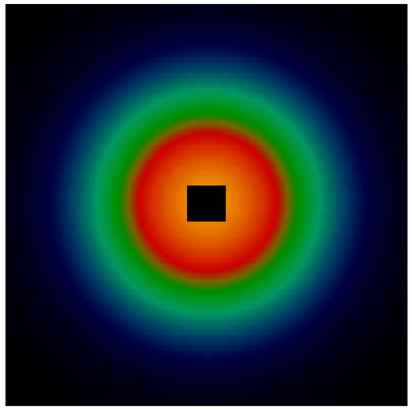
J Kohlbrecher PSI



$$\frac{2\pi}{d} = Q = \frac{4\pi}{\lambda}\sin\left(\theta/2\right)$$

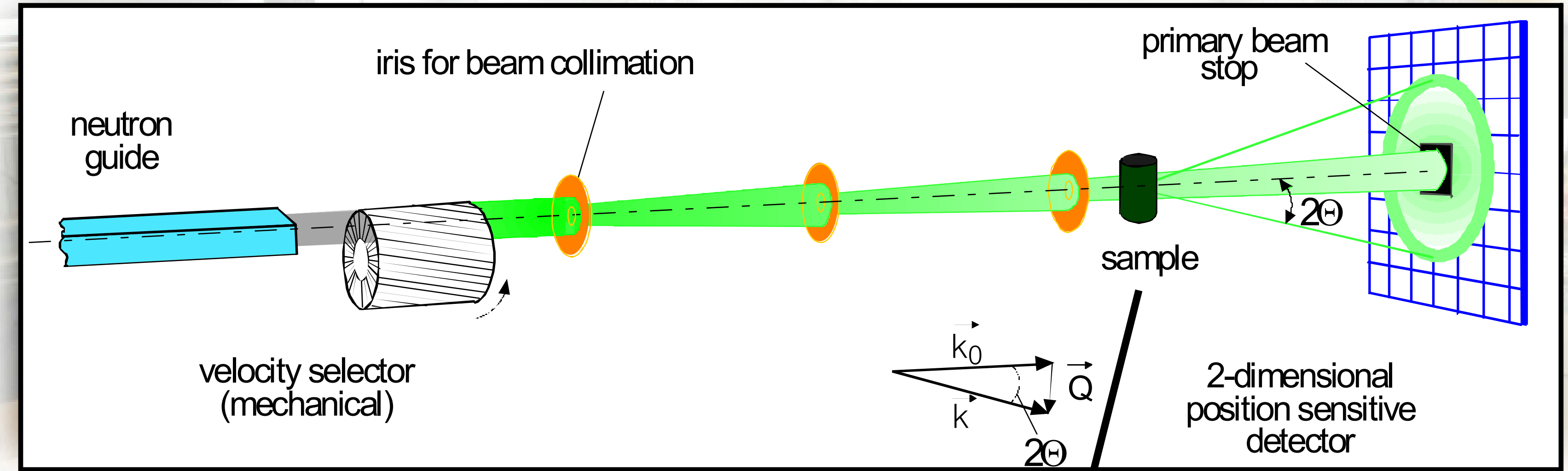
$\lambda \approx 0.5$ nm
d ≈ 10 nm
$\Rightarrow$ $\theta \approx 3$ deg





Small Angle Neutron Scattering

J Kohlbrecher PSI



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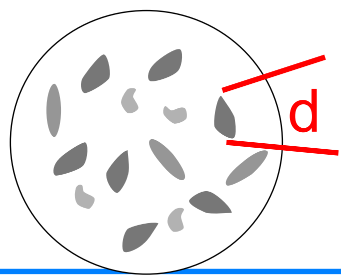
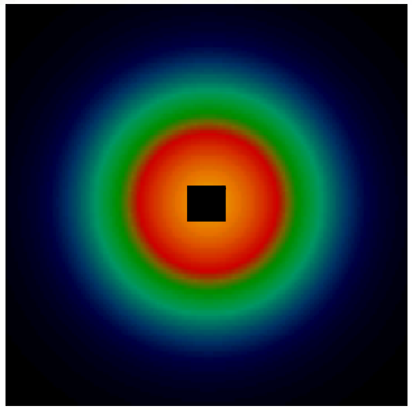
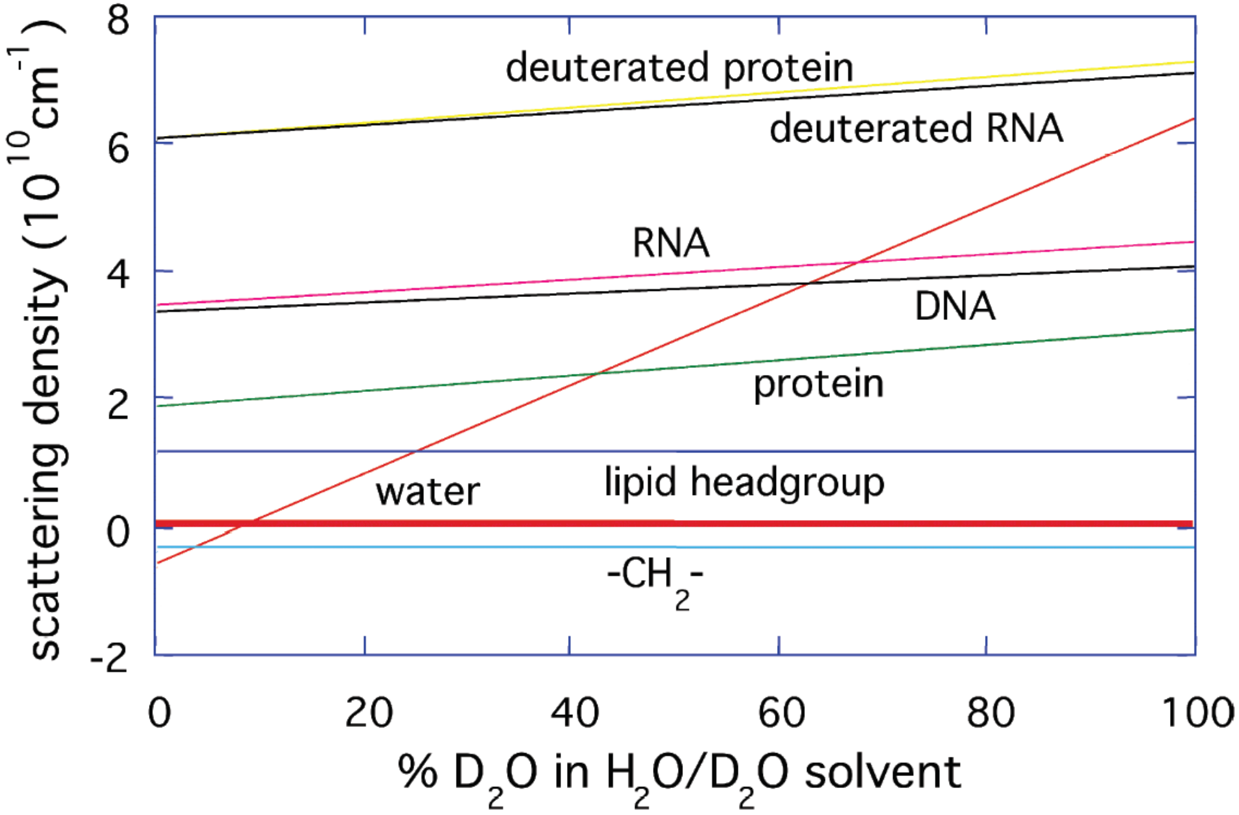


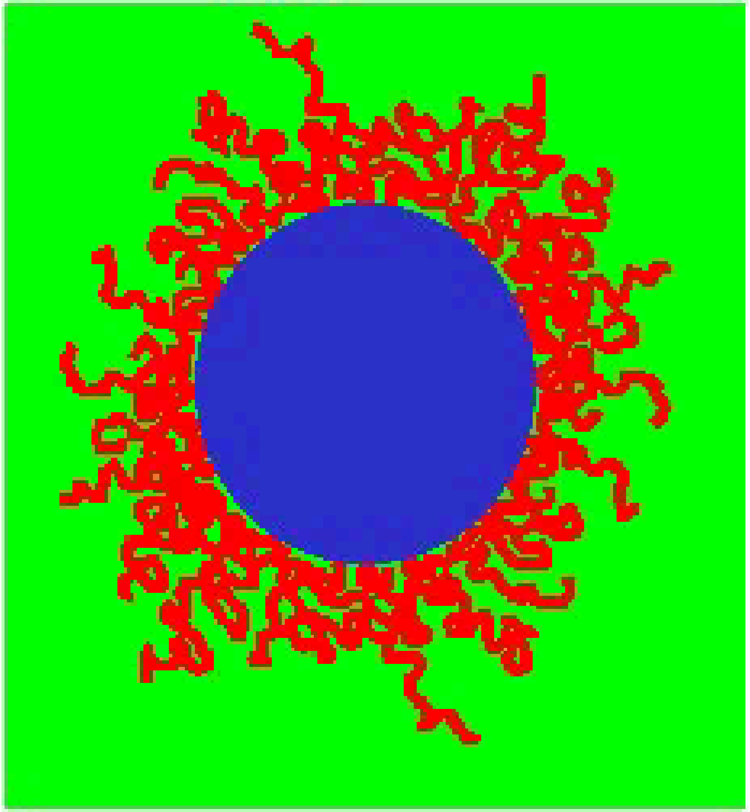


Contrast Variation

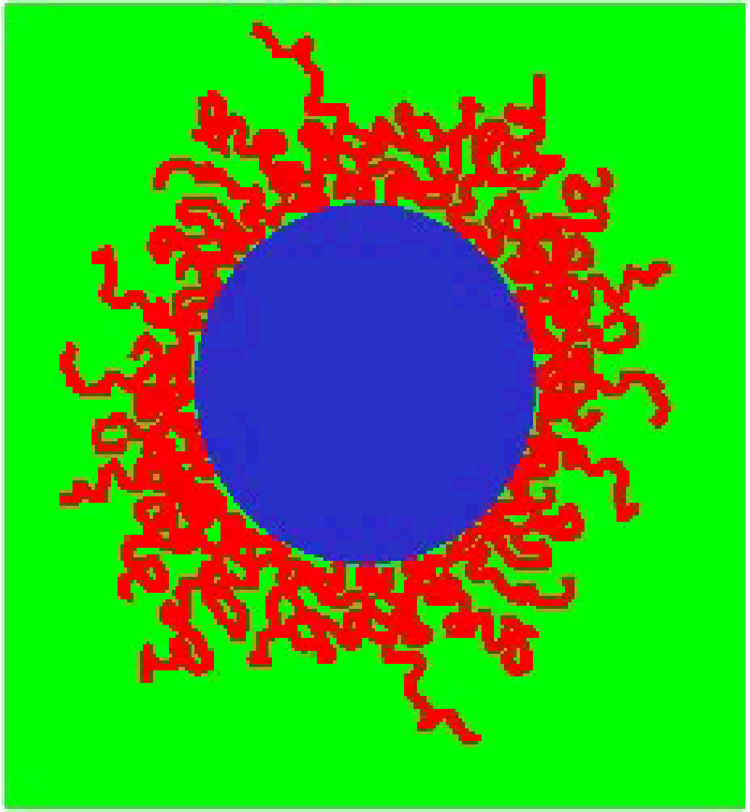
- A different fraction of hydrogen leads to a different scattering length density
- Solvent contrast variation: H_2O/D_2O mixtures match different material at different D_2O percentage



Contrast Variation



matching of core



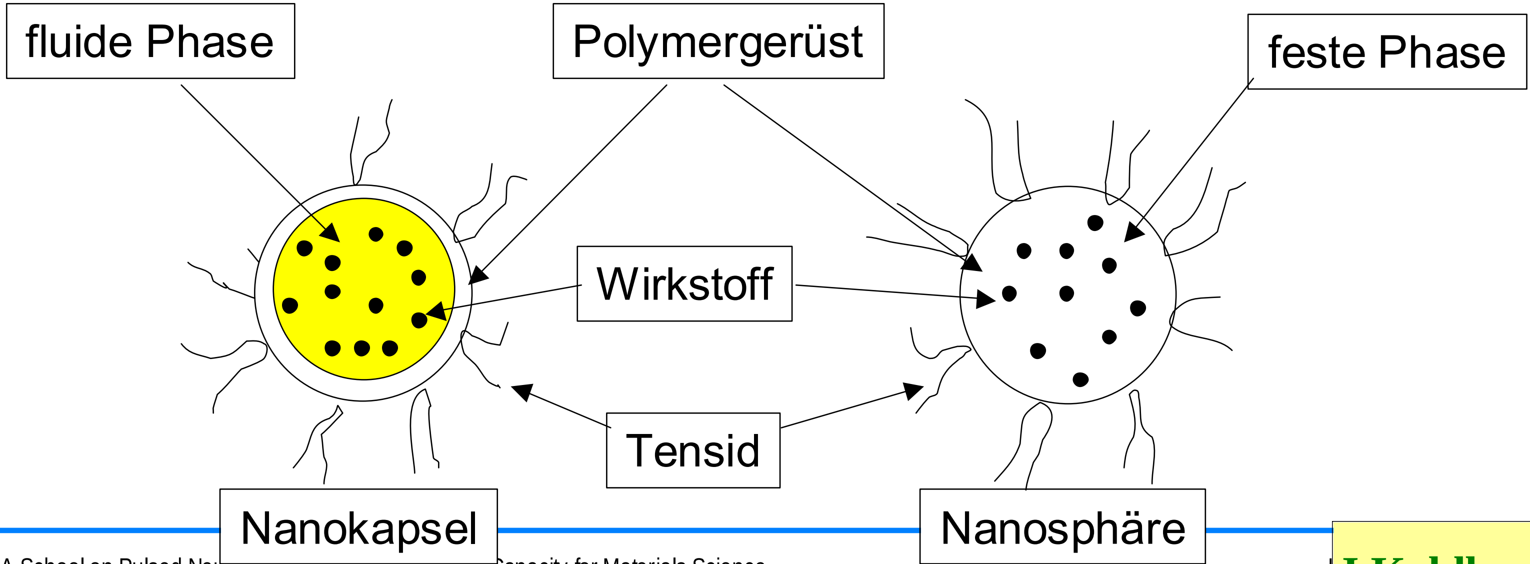
matching of shell

J Kohlbrecher PSI

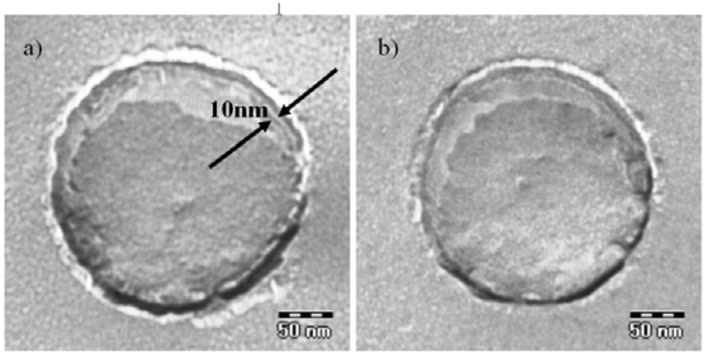
Drug Targeting: Core-Shell Structure of Poly(D,L-lactide) Nanocapsules

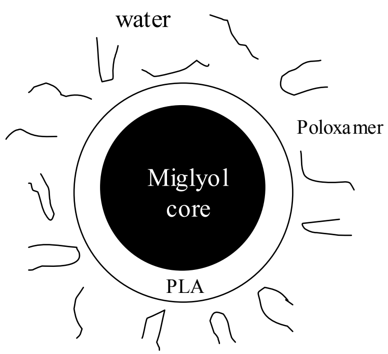
Andrea Rübe[1], Gerd Hause[2], Karsten Mäder[1], Joachim Kohlbrecher[3*]
[1]Institute of Pharmaceutical Technology and Biopharmacy, Martin-Luther-University Halle-Wittenberg
[2]Microscopy Unit, Biocenter of the University, Halle/Saale
[3]Laboratory for Neutron Scattering, Paul Scherrer Institute

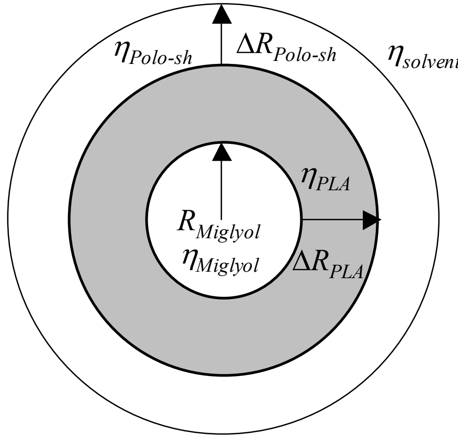
- Einschluss von lipophilen Wirkstoffen in die innere Ölphase möglich
- Tensidschicht umgibt Nanokapseln, um sie im Wasser zu stabilisieren

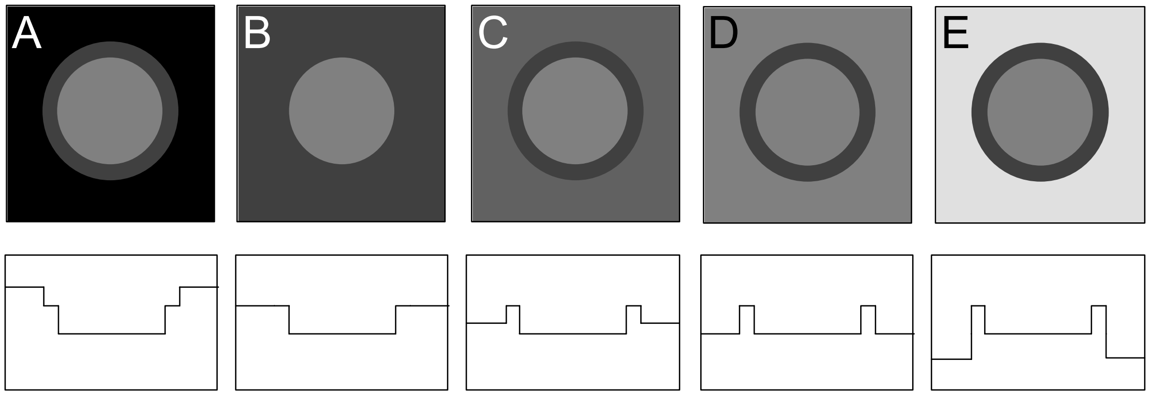


Drug Targeting: Core-Shell Structure of Poly(D,L-lactide) Nanocapsules









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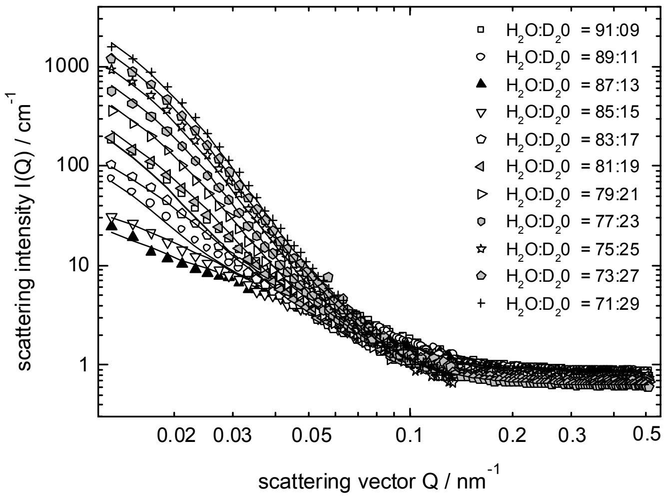
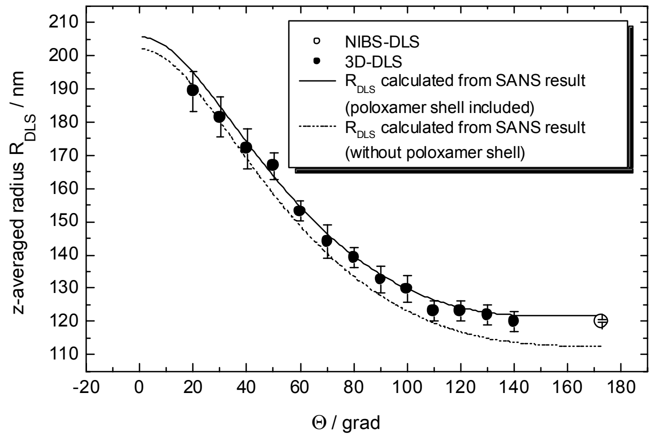
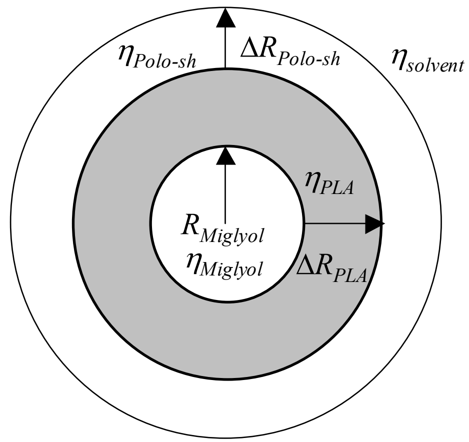
Drug Targeting: Core-Shell Structure of Poly(D,L-lactide) Nanocapsules

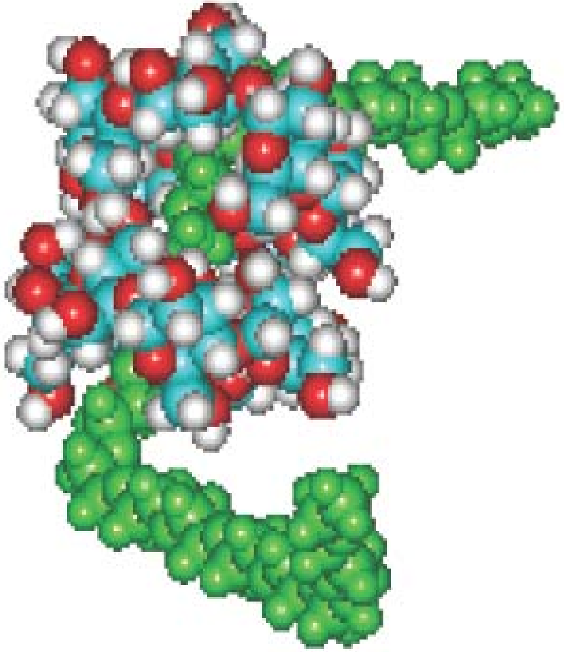




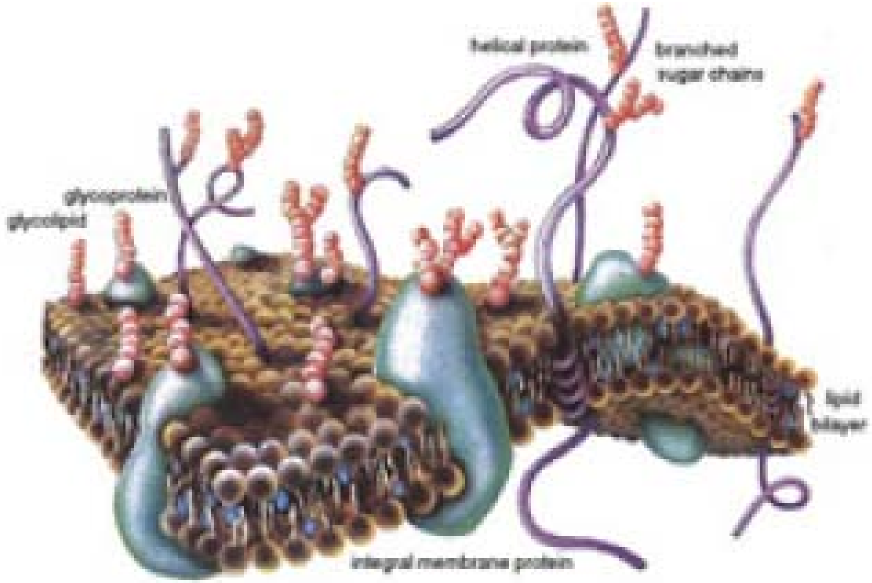


σ = 0.394,
R_0 = 84 nm,
ΔR_{PLA} = 9.8 nm
$\Delta R_{Polo\text{-}sh}$=17 nm
Poloxamer concentration in outer shell of 7%.

From solutions → Membranes

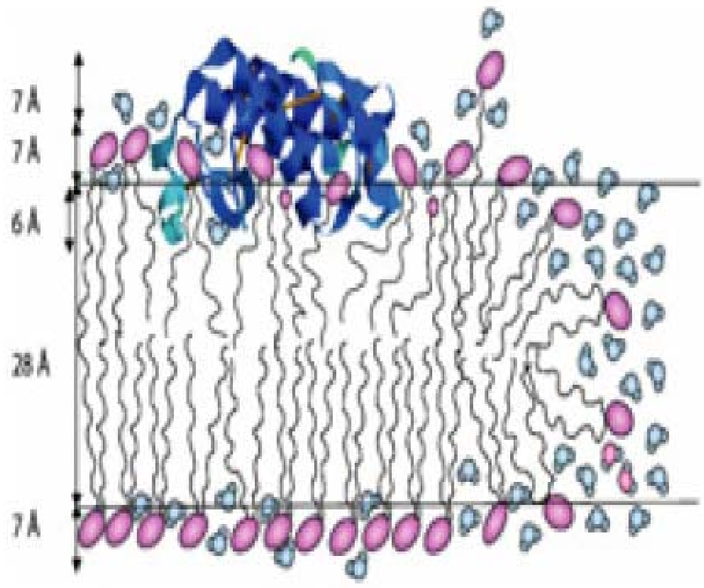


Self assembled polyrotaxanes
(polymer complexes)



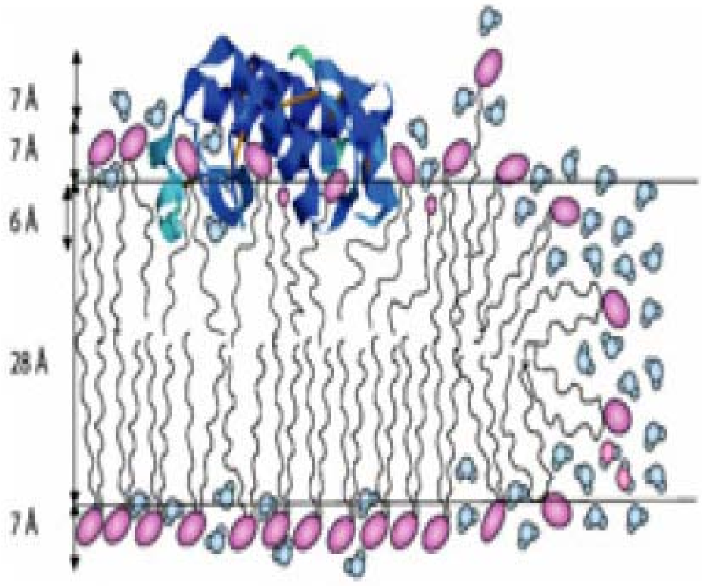
The cell membrane, showing the location of proteins and other cellular material within the phospholipid bilayer

Function ……….



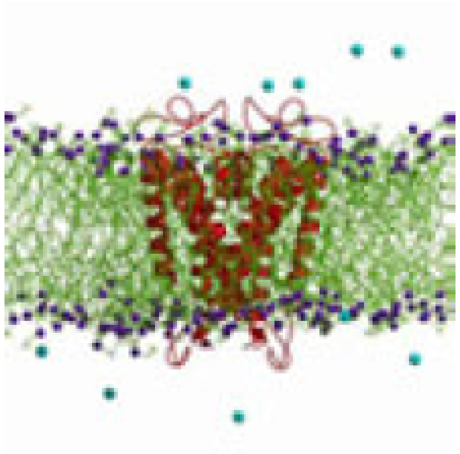
Schematic representation of Phospholipase A2 interacting with a phospholipid bilayer, derived from neutron reflectometry.

Function ....



Schematic representation of Phospholipase A2 interacting with a phospholipid bilayer, derived from neutron reflectometry.

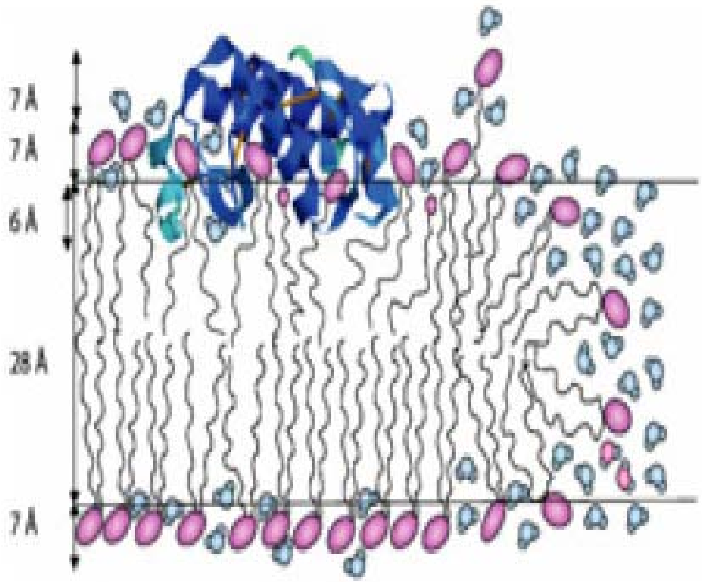
Natural Antibiotics



Molecular structure showing the location of an integral membrane protein.

Function ....

Natural Antibiotics



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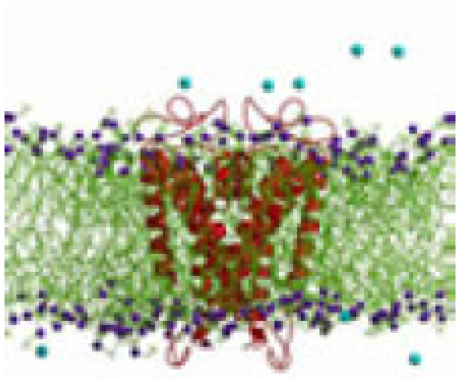
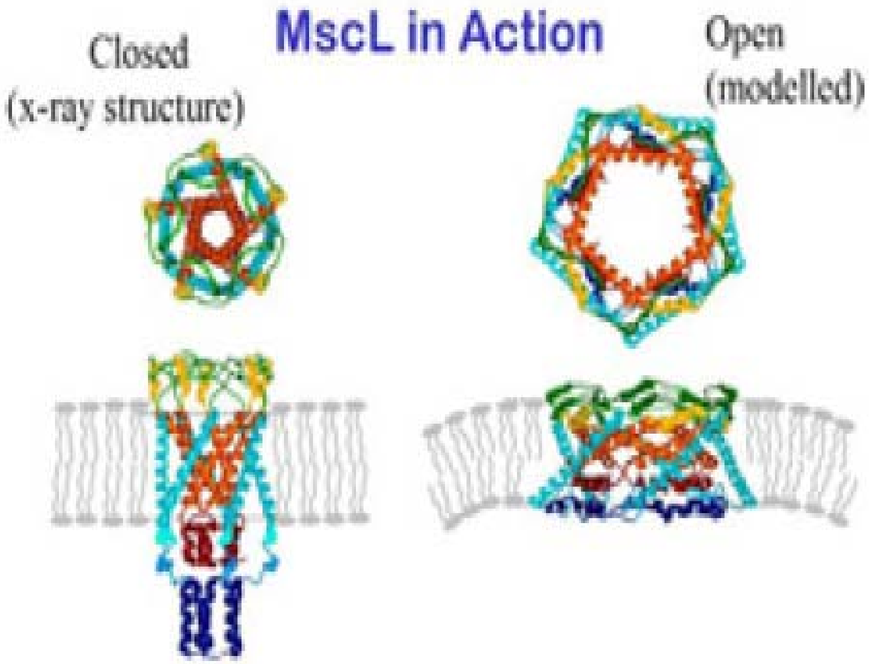


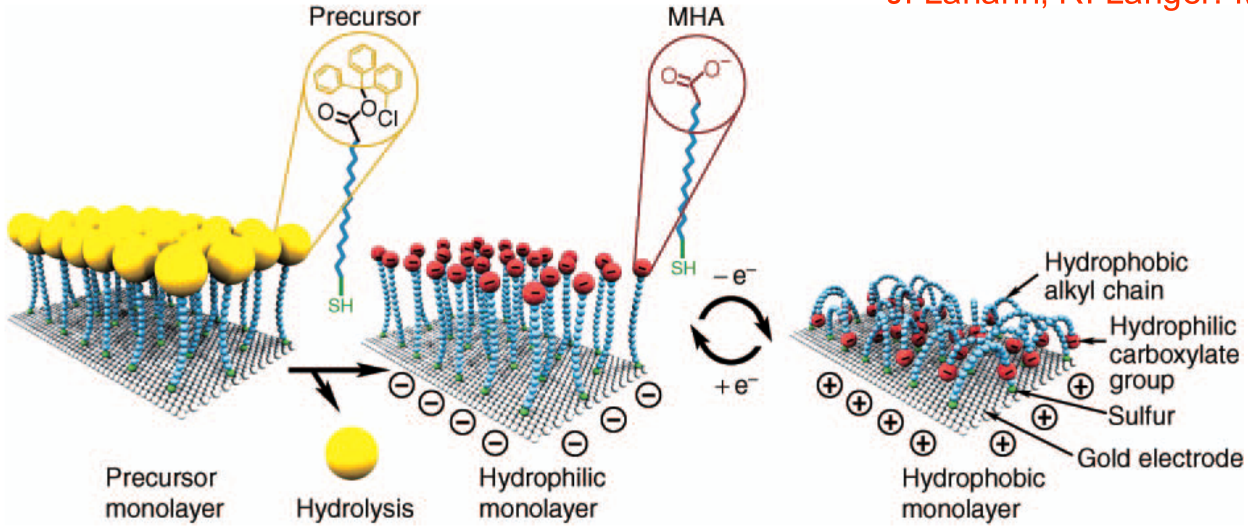


Schematic representation of the proposed mechanism of the MscL channel.

Biomimetics – functional surfaces

Dynamically Controlled Surface Properties (T, pH, Light, V, etc.)

J. Lahann, R. Langer: MRS Bulletin

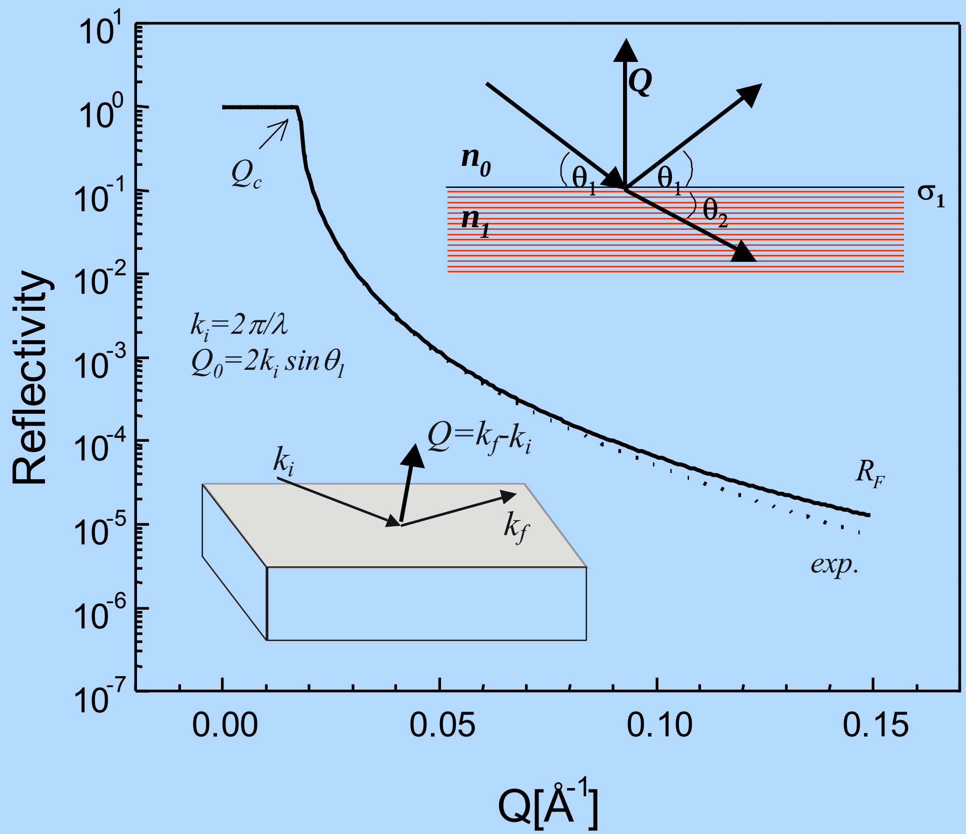


Applications:

- Biosensors
- Microfluidic devices (valves, reservoirs)
- Structural templates for tissue engineering
- Drug delivery
- Study of cell/cell and cell/protein interactions

T Mason, SNS

Biomembranes and Interfaces



Reflectivity of a single interface (Fresnel reflectivity)

$R = r\, r^*$

$r = A'_1/A_1 = (Q_0-Q_1)/(Q_0+Q_1)$ reflection coefficient

with $Q_i = (Q_0^2-Q_c^2)^{1/2}$

$$R_F(Q) = \left|\frac{1-[1-(Q_c/Q_0)^2]^{1/2}}{1+[1-(Q_c/Q_0)^2]^{1/2}}\right|^2$$

for $Q_0 > Q_c$

$$R_F(Q) \approx (Q_c/Q_0)^4$$

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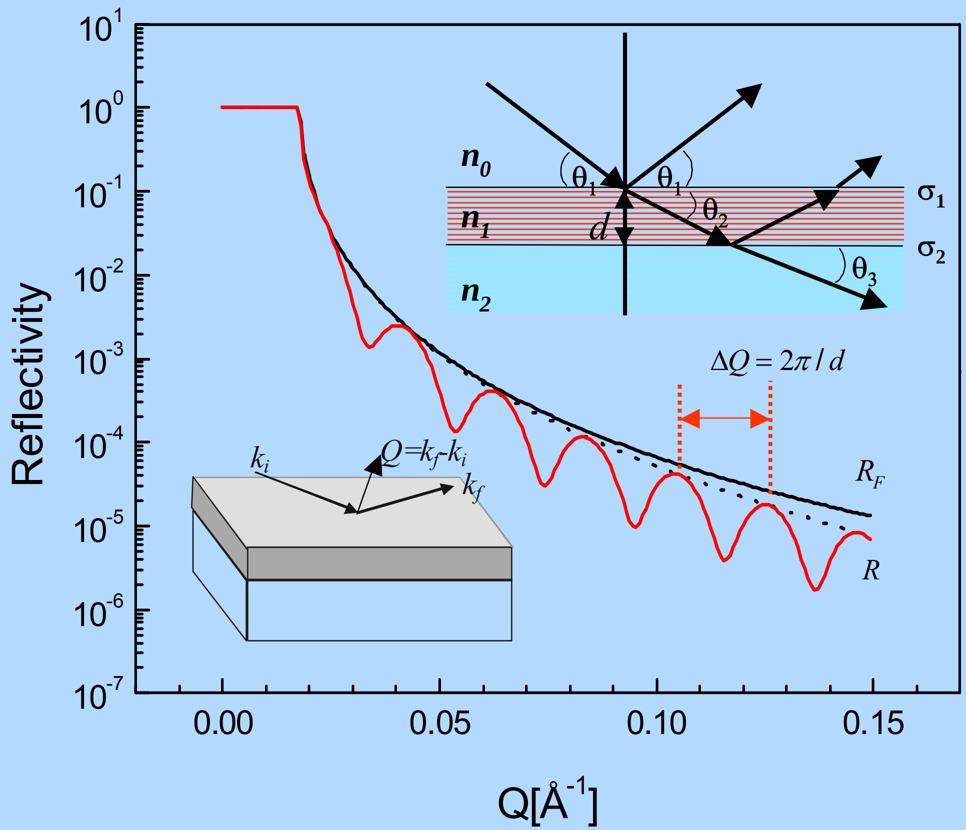
Biomembranes and Interfaces



Reflectivity of two interfaces

$$R(Q) = \frac{r_1^2 + r_2^2 + 2 r_1 r_2 \cos(2Q_1 d)}{1 + r_1^2 r_2^2 + 2 r_1 r_2 \cos(2Q_1 d)}$$

with thickness $d = 2\pi/\Delta Q$

in kinematic theory

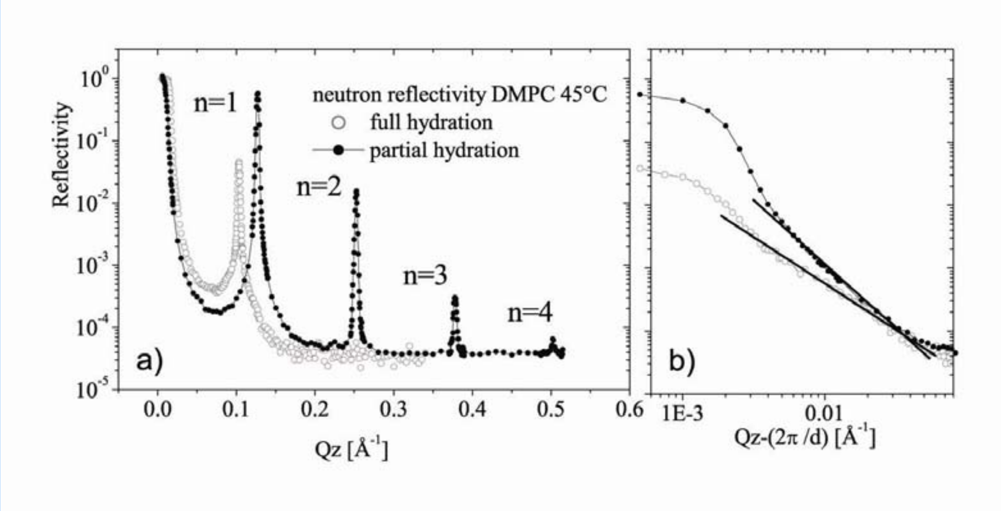
$$r = \frac{(k_c^2)^2}{Q_0^4} \left| \int \frac{d\rho}{dz} \cdot \exp(iQ_0 z)\, dz \right|^2$$

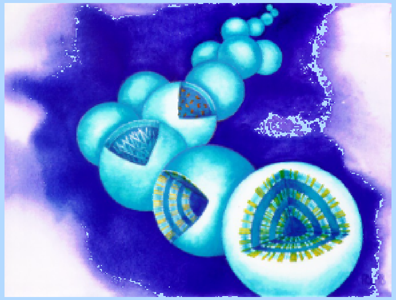
reflectivity of two interfaces

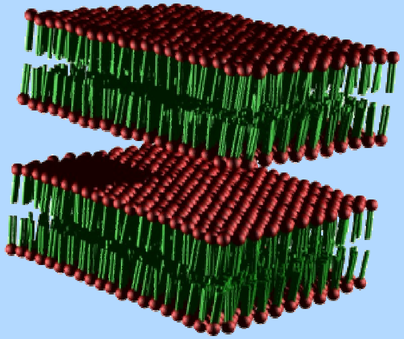
$$R(Q) = \frac{(k_c^2)^2}{Q^4} \left[\begin{array}{l} \Delta\rho_1 \cdot \exp(-Q^2\sigma_1^2) + \Delta\rho_2 \cdot \exp(-Q^2\sigma_2^2) \\ + \Delta\rho_3 \cdot \exp(-Q^2(\sigma_1^2 + \sigma_2^2)/2) \cdot \cos(Q\mathrm{d}) \end{array} \right]$$

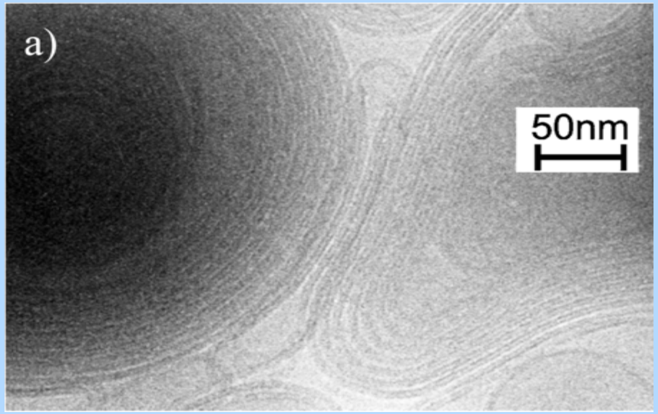
with parameters $d,\ \sigma,\ \Delta\rho$

Biomembranes





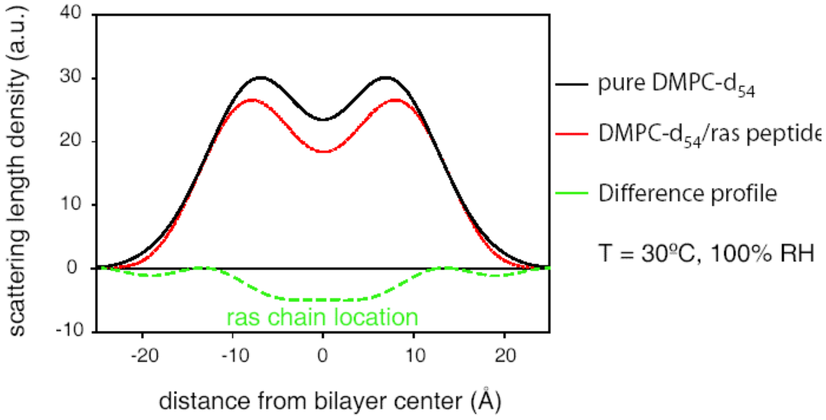


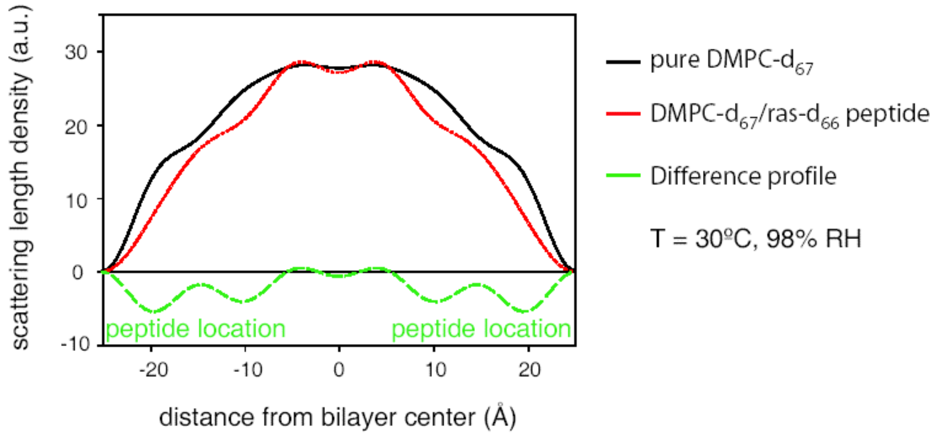


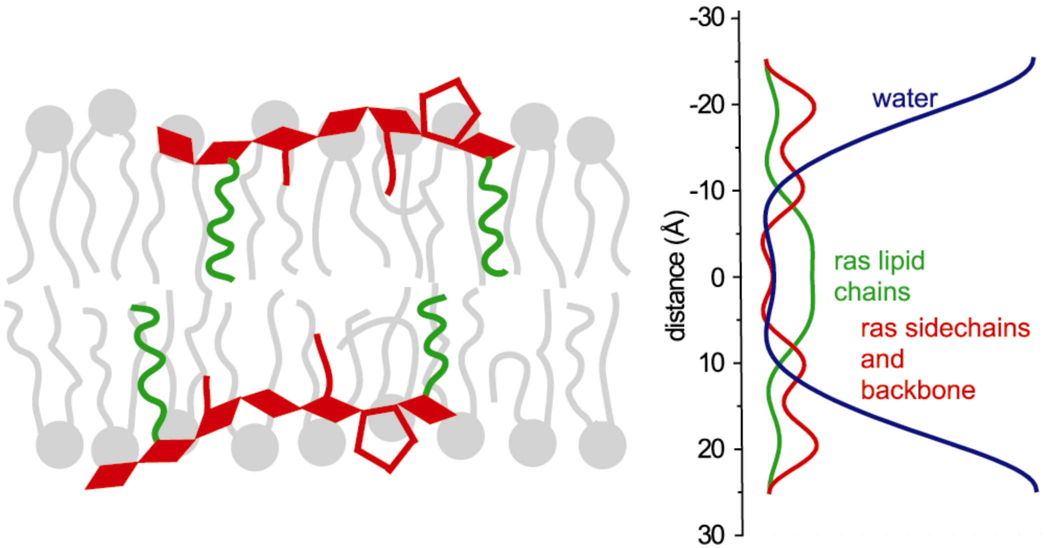
multilamellar vesicles

(from B. Klösgen in Lipid Bilayers - Structure and Interactions)

Membrane Binding of Lipidated N-ras Peptide







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(D. Huster et al., JACS, 125, 2003, 4070)

Biomembranes and Interfaces

Anchoring of Recombinant Proteins to Functionalized Phospholipid Monolayers

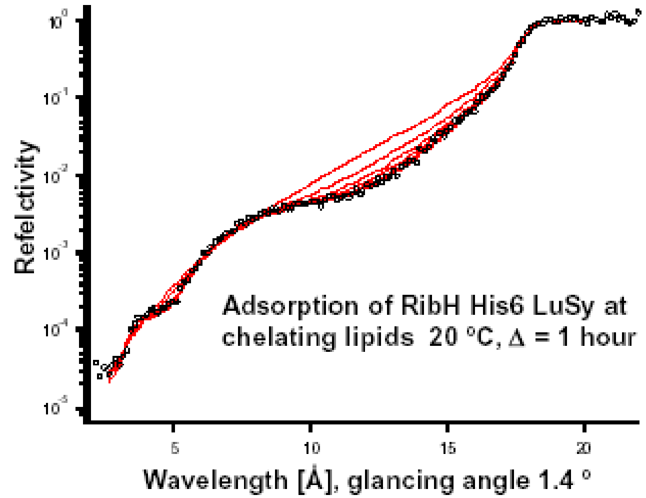

Figure 1. Reflectivity data obtained during the adsorption of LuSy to a Ni Chelator covered surface. The lines correspond to the best fits of the neutron reflectivity data sets, plotted over wavelength. The time distance between two sets of data is one hour.

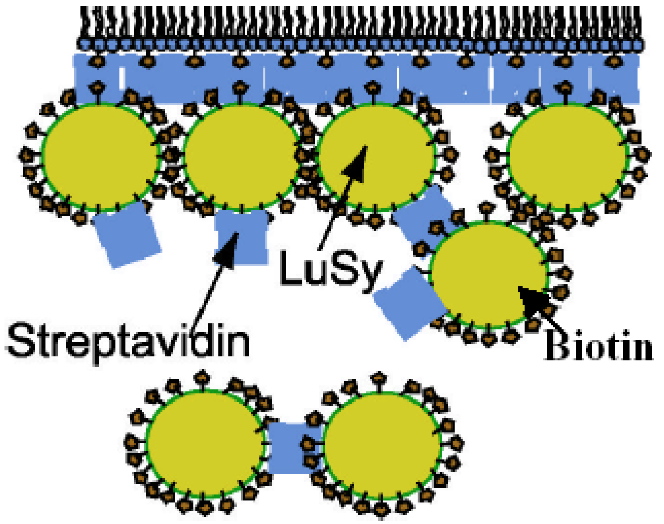

Figure 4. Model of multilayers to fit the data of biotin Lusy adsorbed to a streptavidin interface

M. Tristl et al., LLB Scientific Report 1999-2000, 100

Biomembranes

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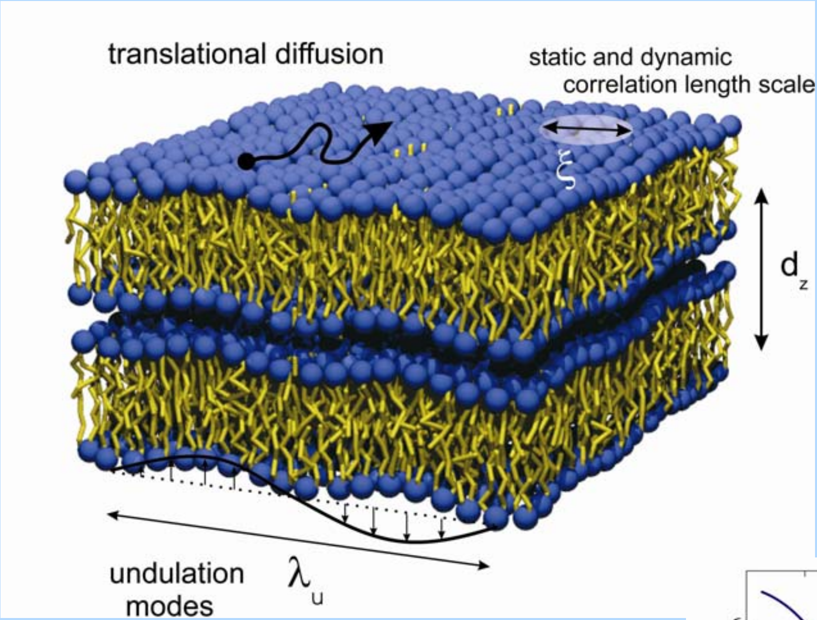
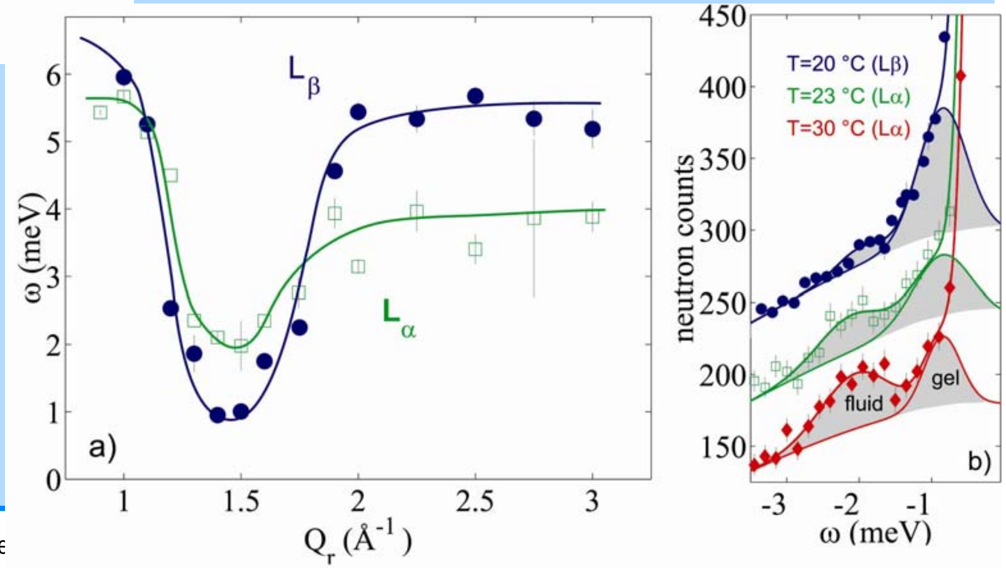
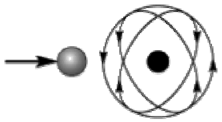


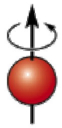


PAUL SCHERRER INSTITUT PSI

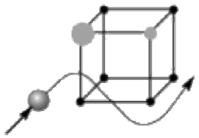
Uniqueness of Neutrons



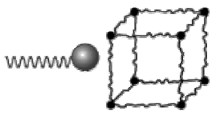
1. Neutrons see the Nuclei



2. Neutrons see Elementary Magnets

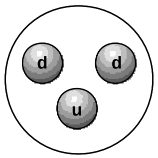


3. Neutrons see Light Atoms next to Heavy Ones



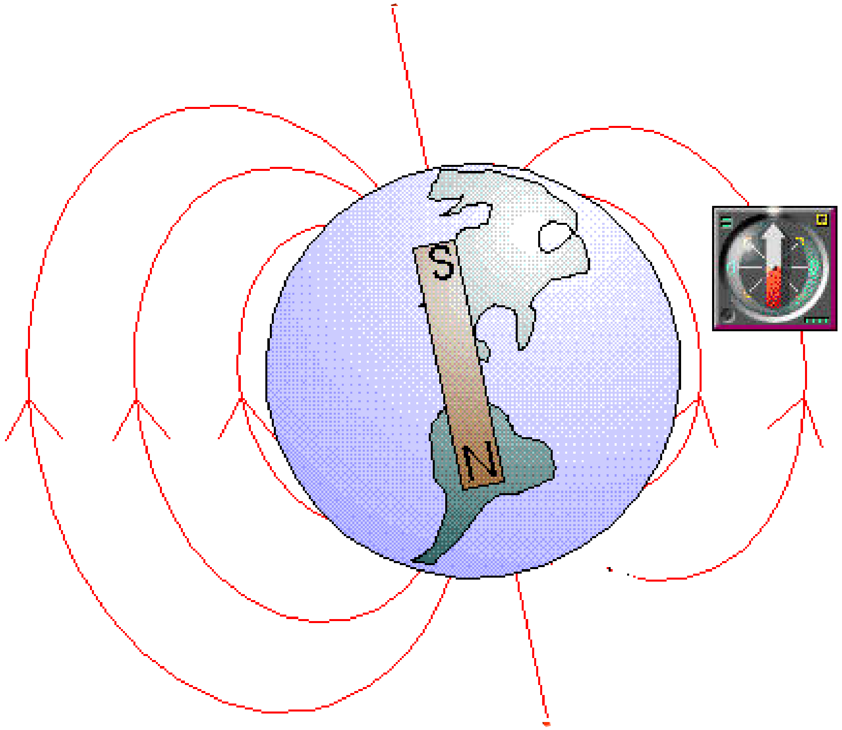
4. Neutrons measure the Velocity of Atoms

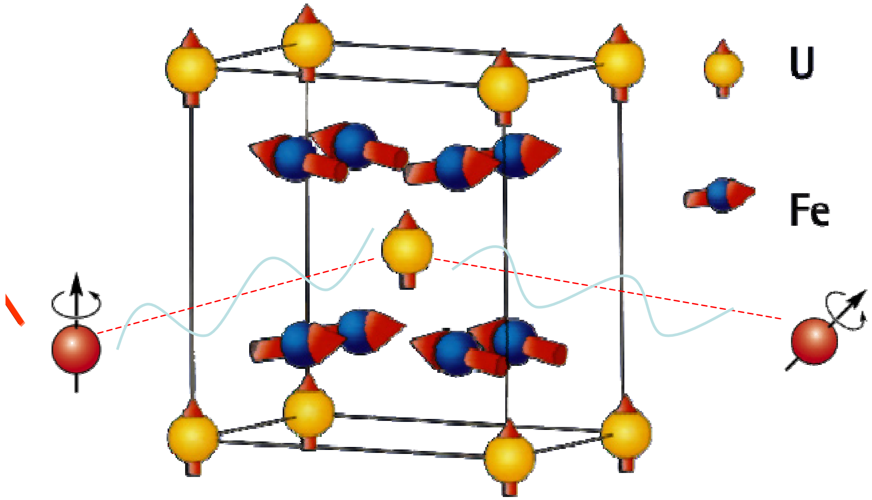
5. Neutrons penetrate deep into Matter



6. Neutrons are Elementary Particles

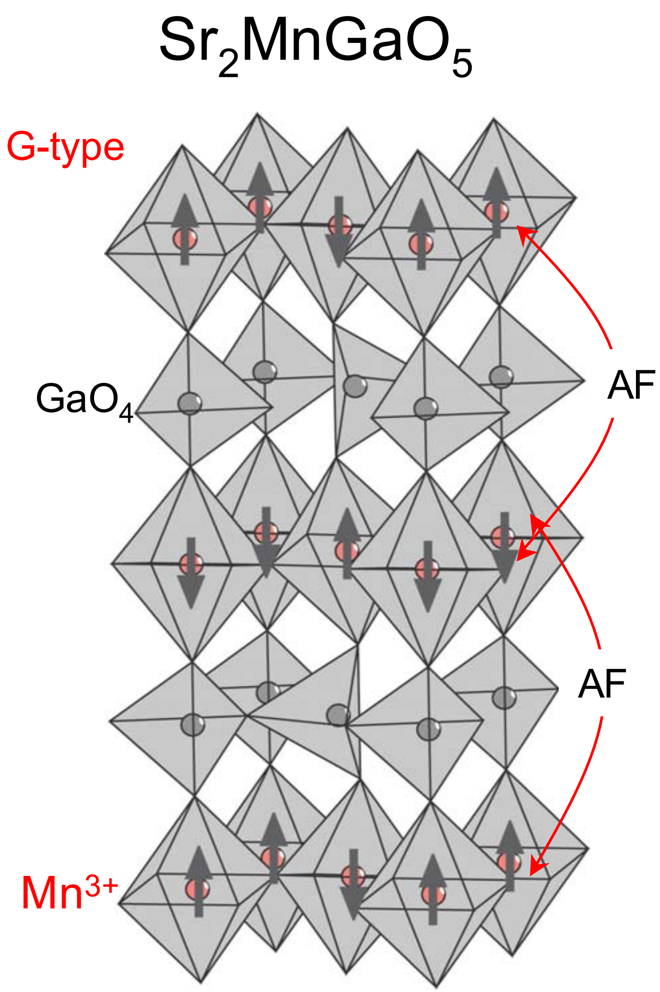
Neutrons see Elementary Magnets

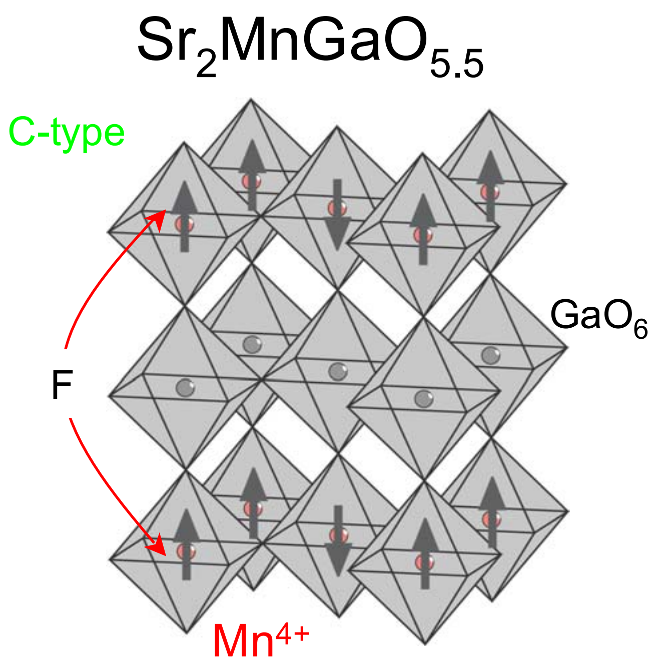




Nearly all what we know about magnetic structures comes from neutrons.

Magnetic and crystal structures





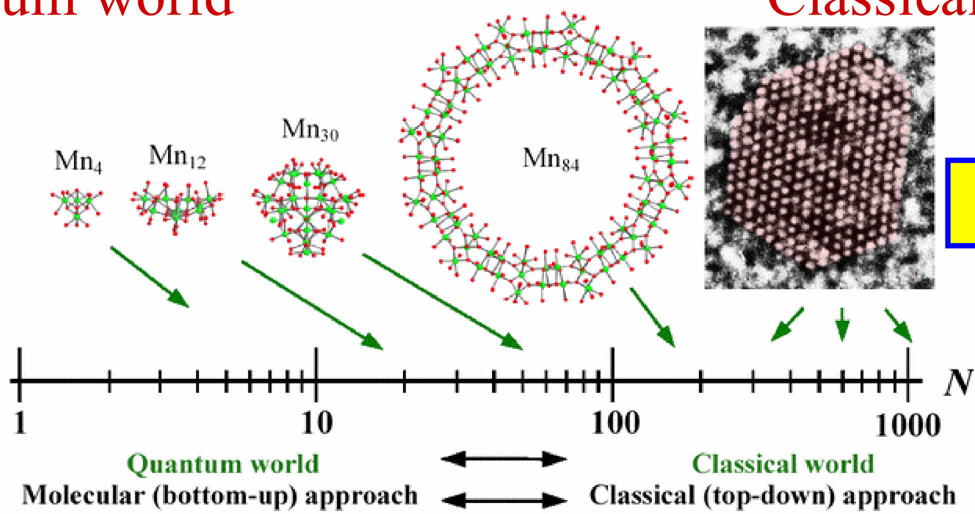
Pomjakushin,V.Yu., Balagurov,A.M., Elzhov,T.V., Sheptyakov,D.V., Fischer,P., Khomskii,D.I., Yushankhai,V.Yu., Abakumov,A.M., Rozova,M.G., Antipov,E.V., Lobanov,M.V., Billinge,S. "Atomic and magnetic structures, disorder effects, and unconventional superexchange interactions in A2GaMnO5+x (A=Sr,Ca) oxides of layered brownmillerite-type structure", Phys. Rev. B 66, 184412 (2002)

V. Pomjakushin PSI

From the classical to the quantum world

Quantum world

Classical world



A. J. Tasiopoulos *et al.*, Angew. Chem. Int. Ed. **43**, 2117 (2004)

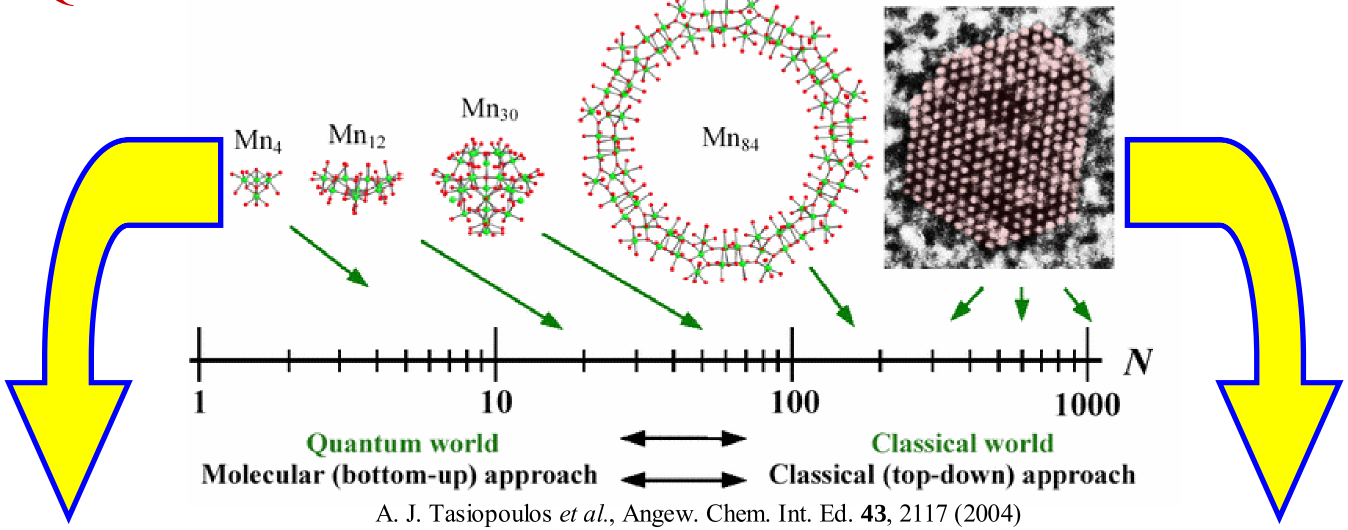
macroscopic behaviour
averaged properties
applications

Christian Rüegg PSI/UCL

From the classical to the quantum world

Quantum world

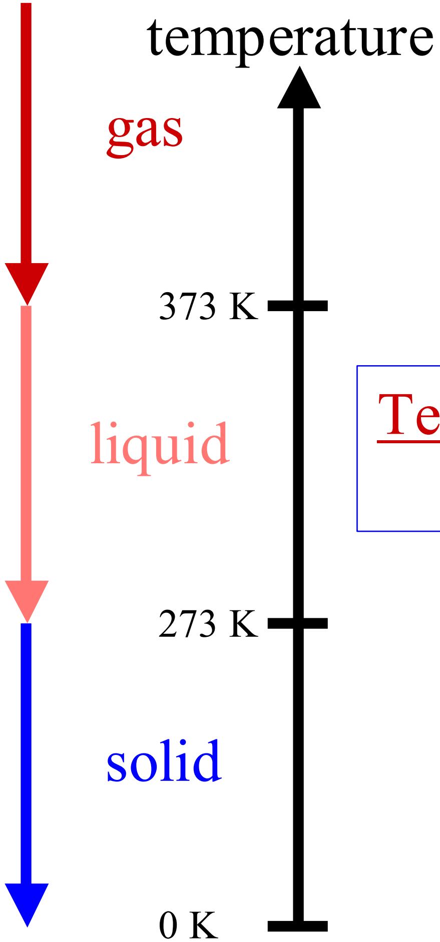
Classical world



microscopic behaviour
individual properties
basic concepts

macroscopic behaviour
averaged properties
applications

Classical phase transitions



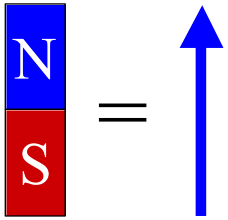
<u>Temperature</u> drives classical phase transitions

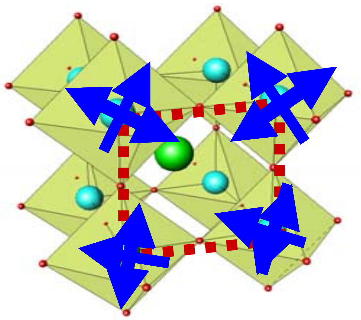
Christian Rüegg PSI/UCL

Phase transitions in classical magnets

<u>Temperature</u> drives classical magnets to an ordered state

temperature



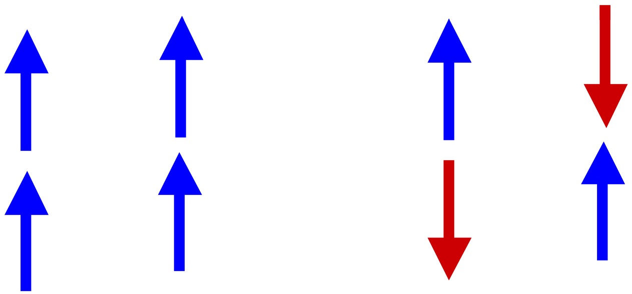


Néel or Curie temperature

0 K

Interactions stronger than disorder by temperature

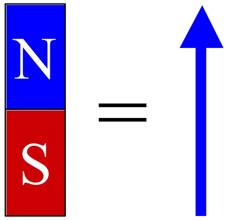
Ferromagnet   Antiferromagnet

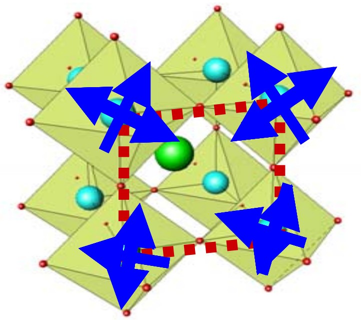


Christian Rüegg PSI/UCL

Phase transitions in classical magnets

temperature





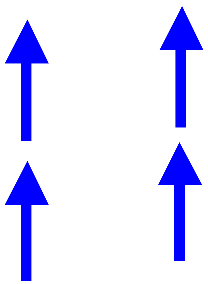
Temperature drives classical magnets to an ordered state

Néel or Curie temperature

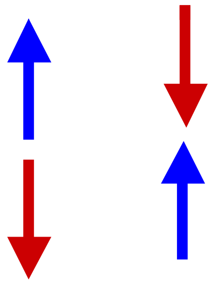
0 K

Interactions stronger than disorder by temperature

Ferromagnet

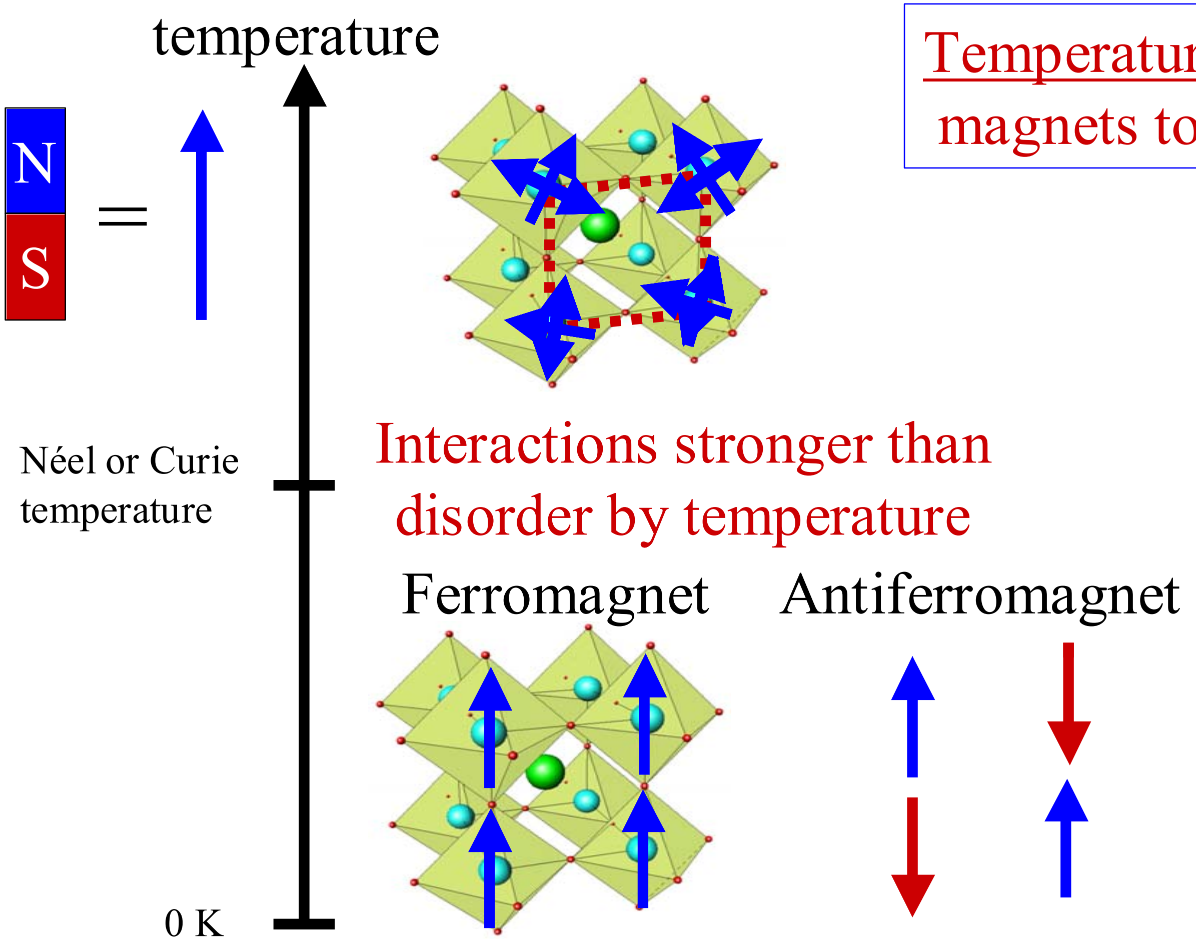


Antiferromagnet



Phase transitions in classical magnets

Temperature drives classical magnets to an ordered state



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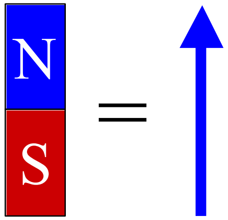
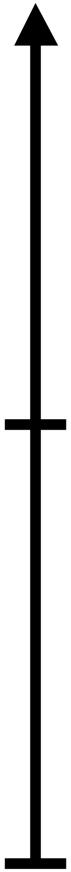
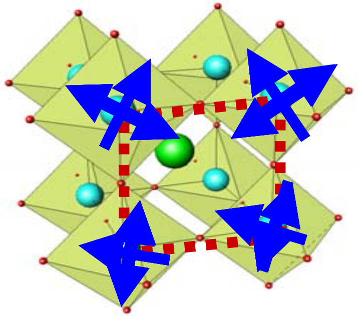
Phase transitions in classical magnets

Temperature drives classical magnets to an ordered state

temperature



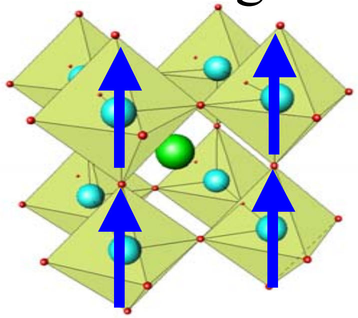




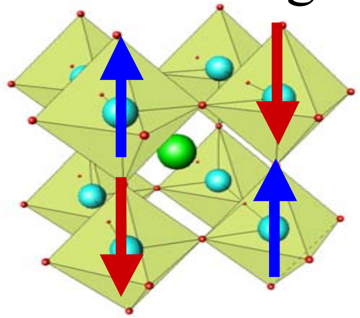
Néel or Curie temperature

Interactions stronger than disorder by temperature

Ferromagnet



Antiferromagnet



0 K

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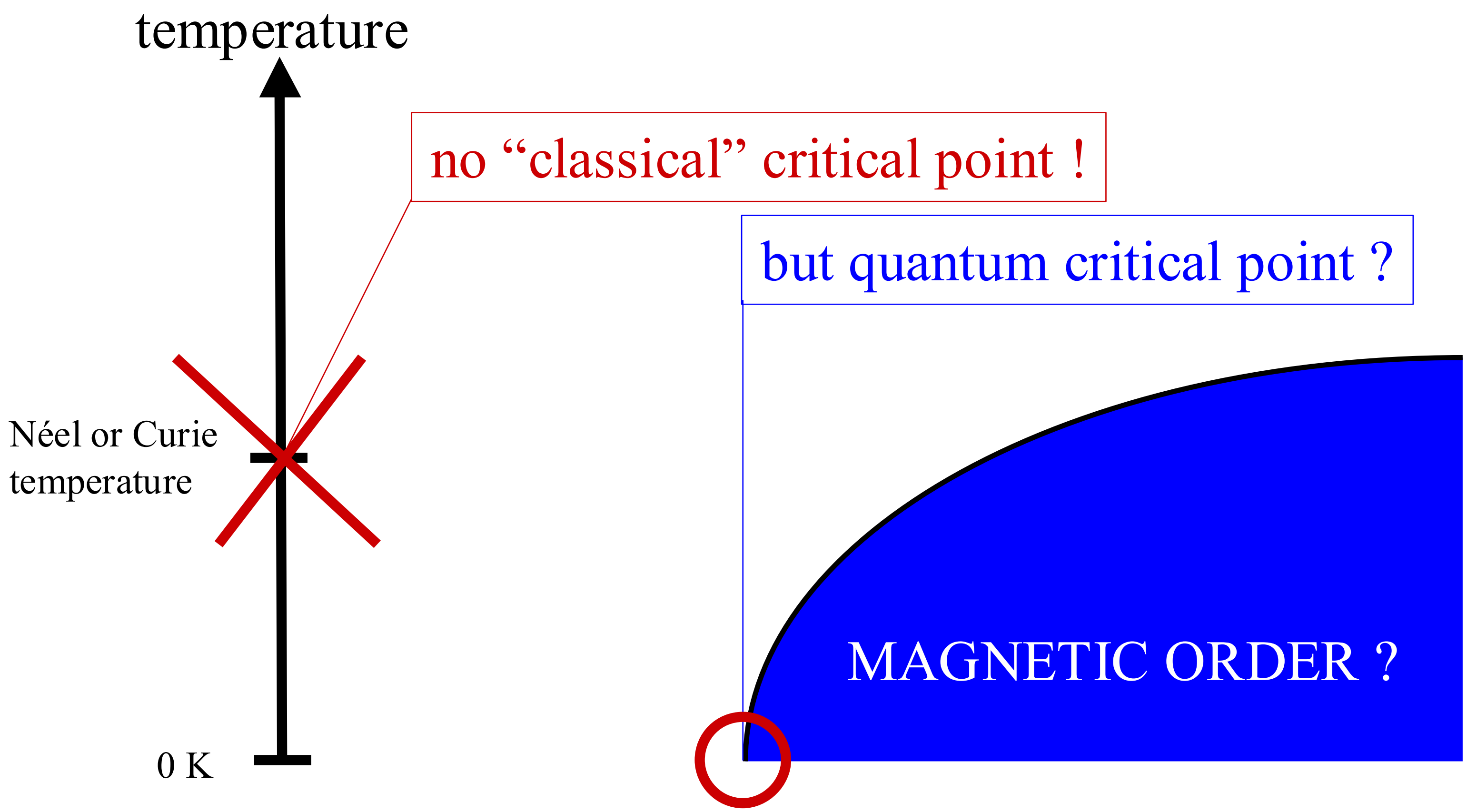
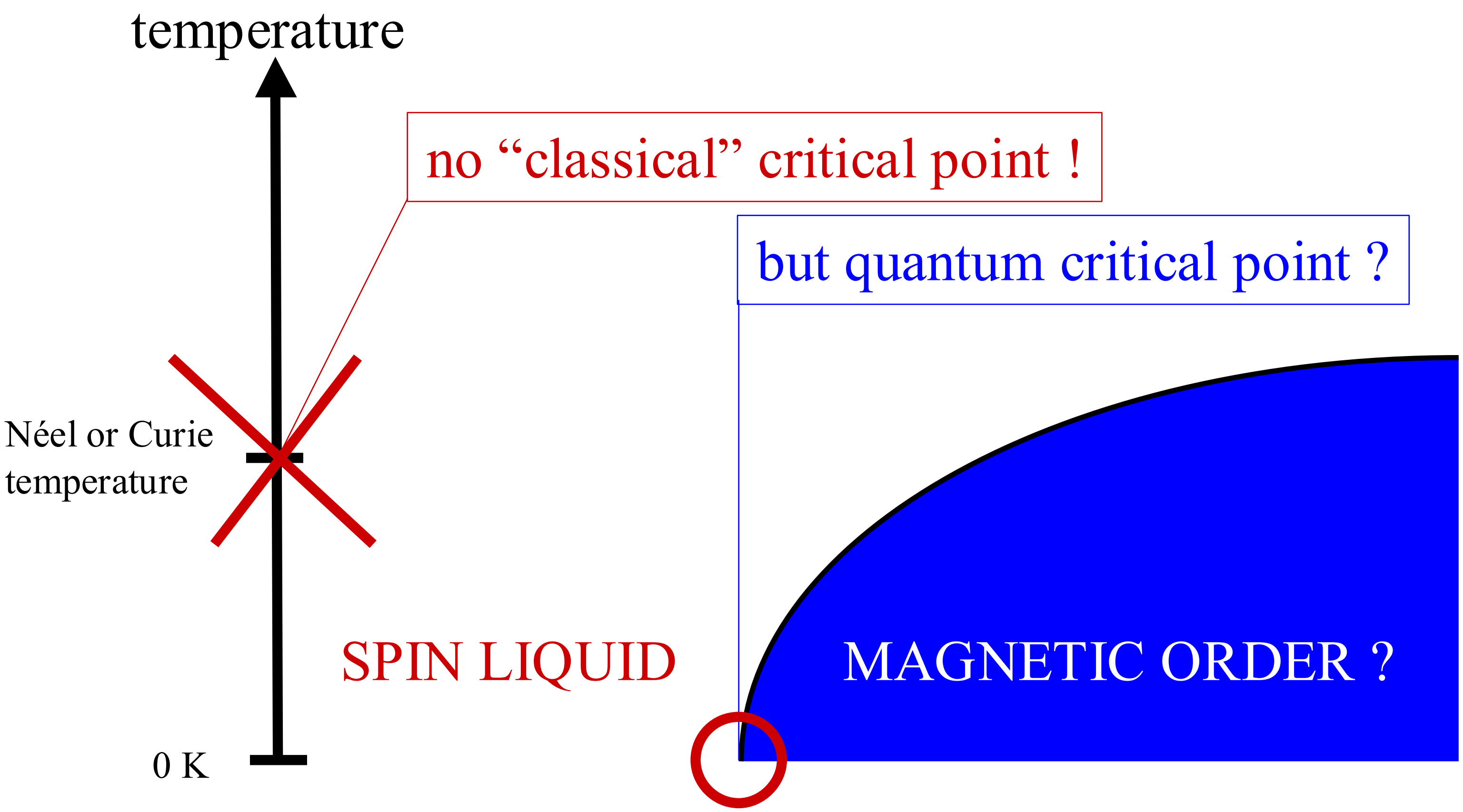
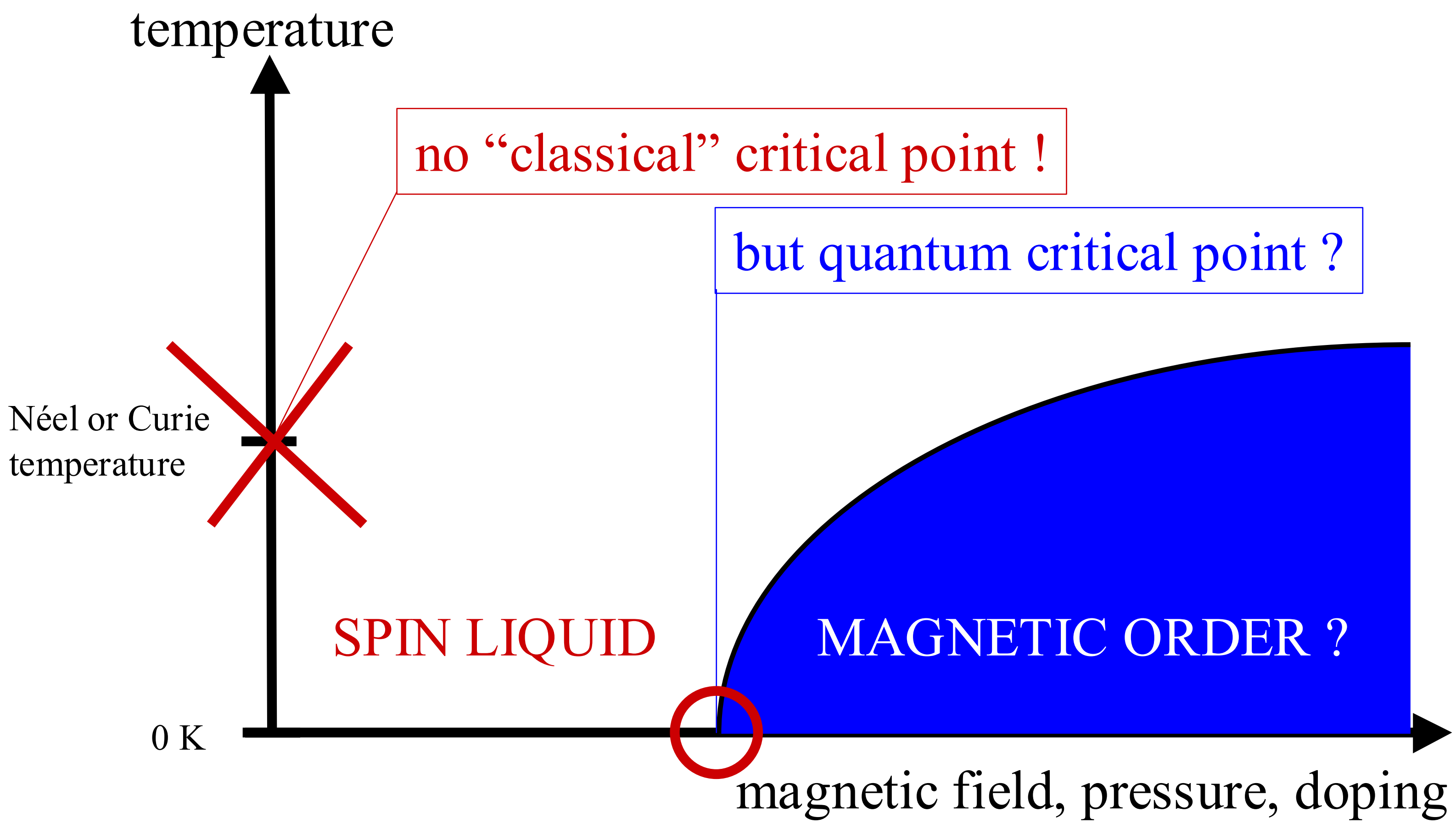
Quantum phase transition



Quantum phase transition

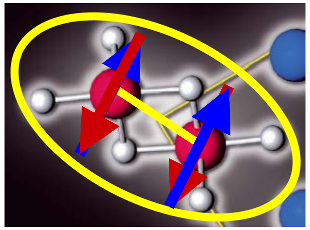


Quantum phase transition



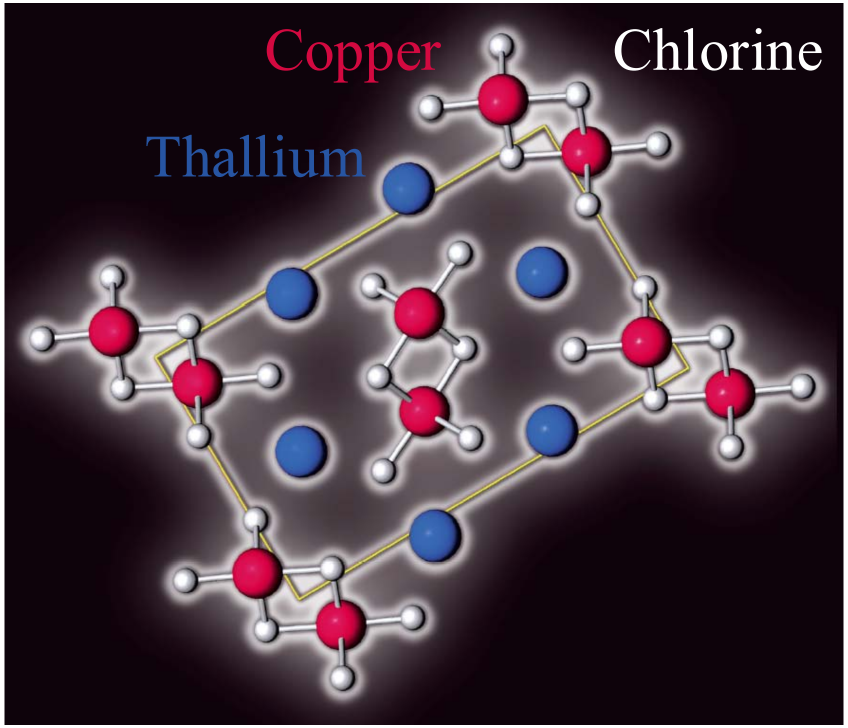
Our quantum model system

Dimer spin system $TlCuCl_3$



- antiferromagnetic
- fluctuating moments
- no magnetic order
- “singlet” ground state

SPIN LIQUID



Christian Rüegg PSI/UCL

Our quantum model system

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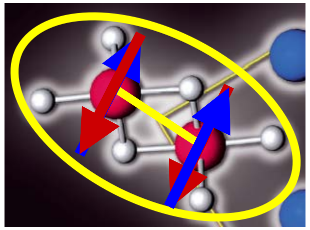

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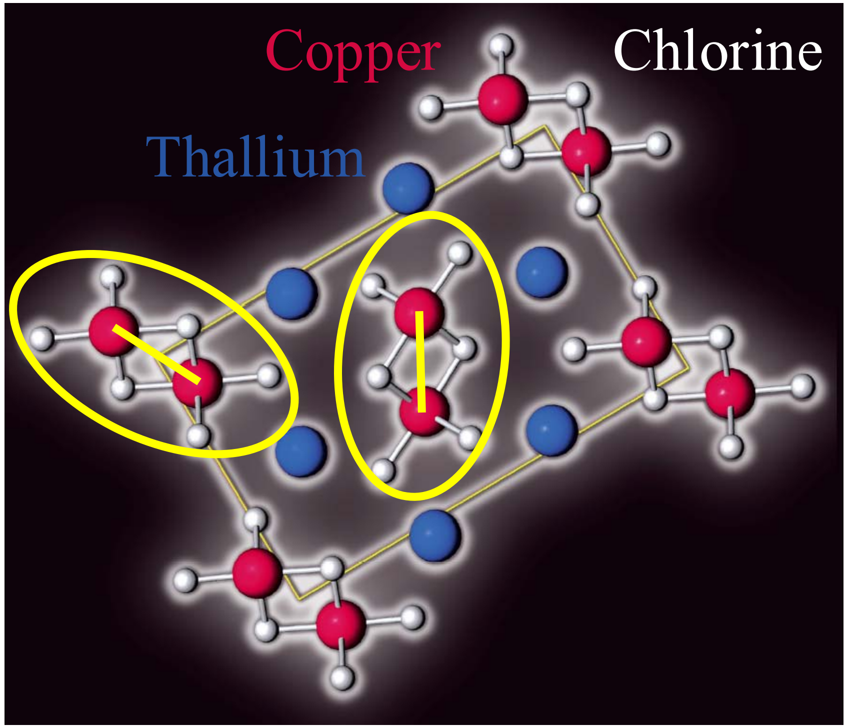

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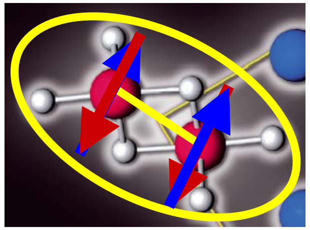

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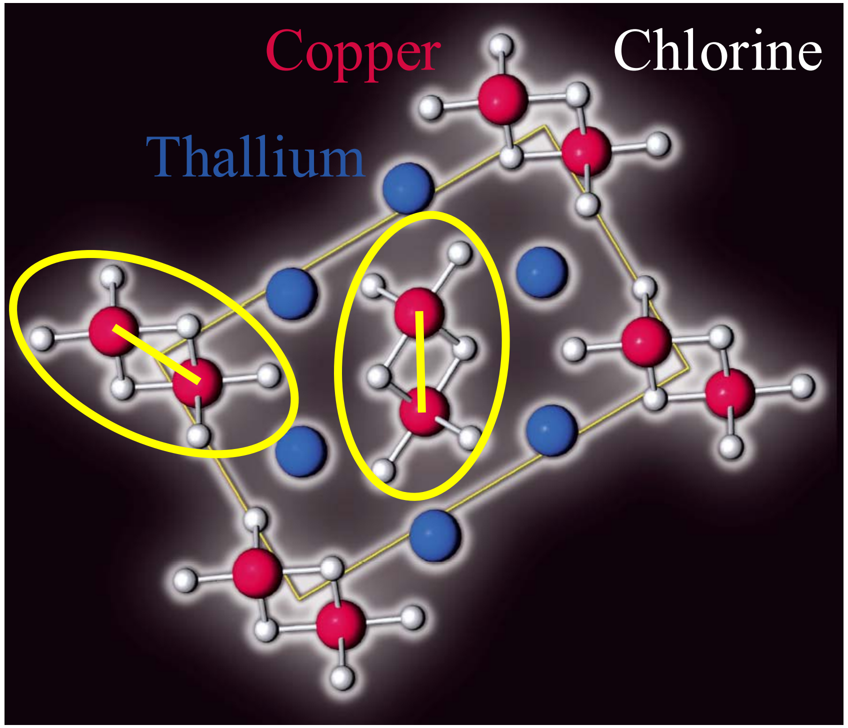

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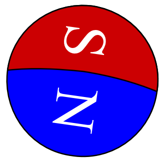
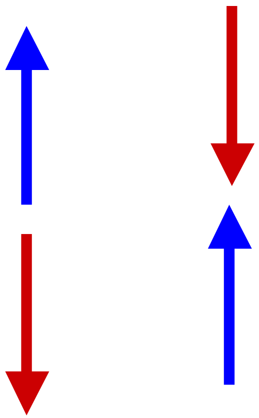
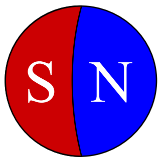
Understanding the ground state

Christian Rüegg PSI/UCL



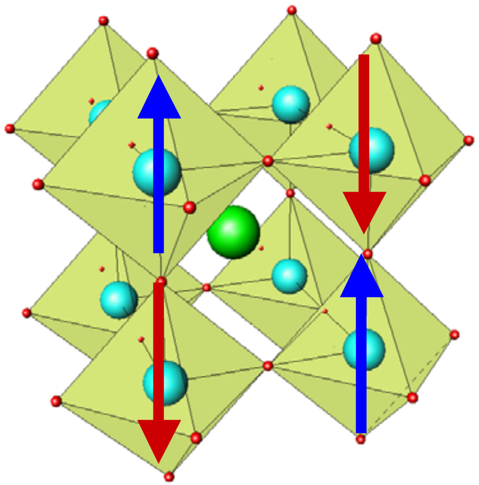


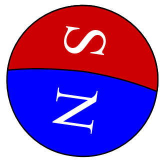
Neutron



Understanding the ground state

Christian Rüegg PSI/UCL





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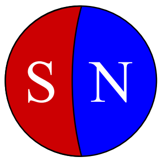
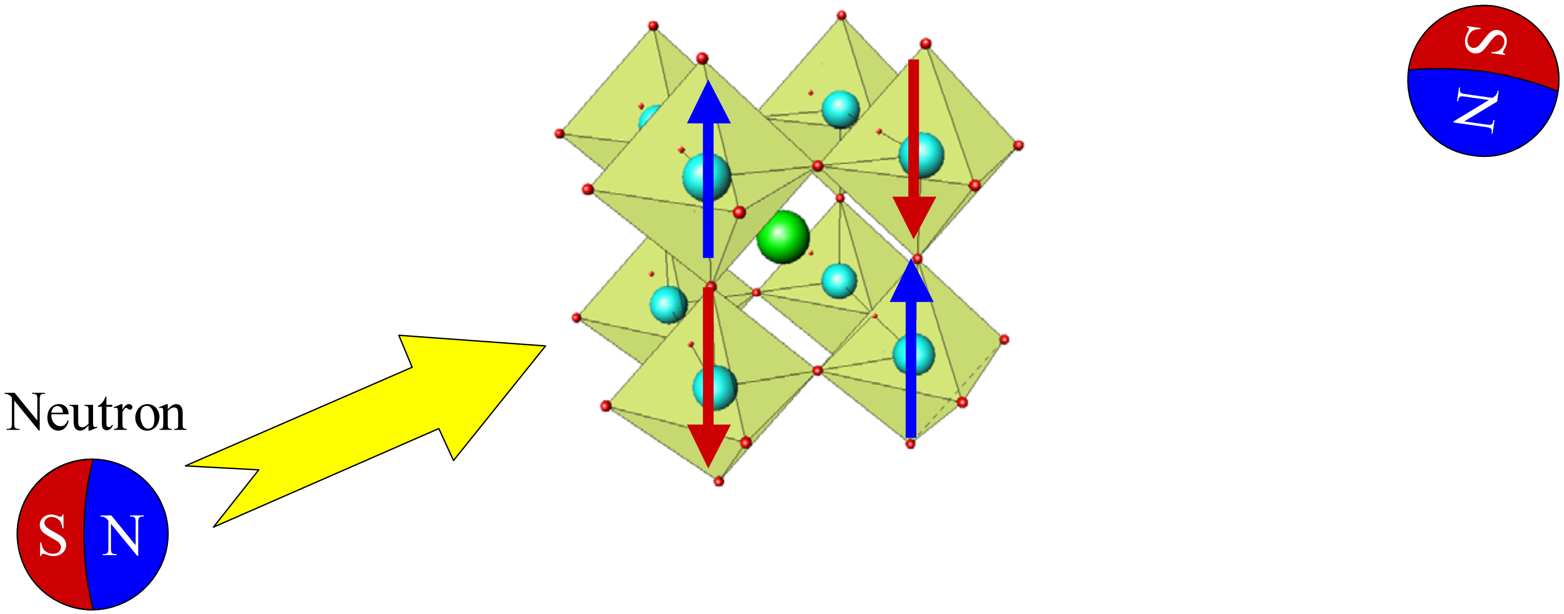


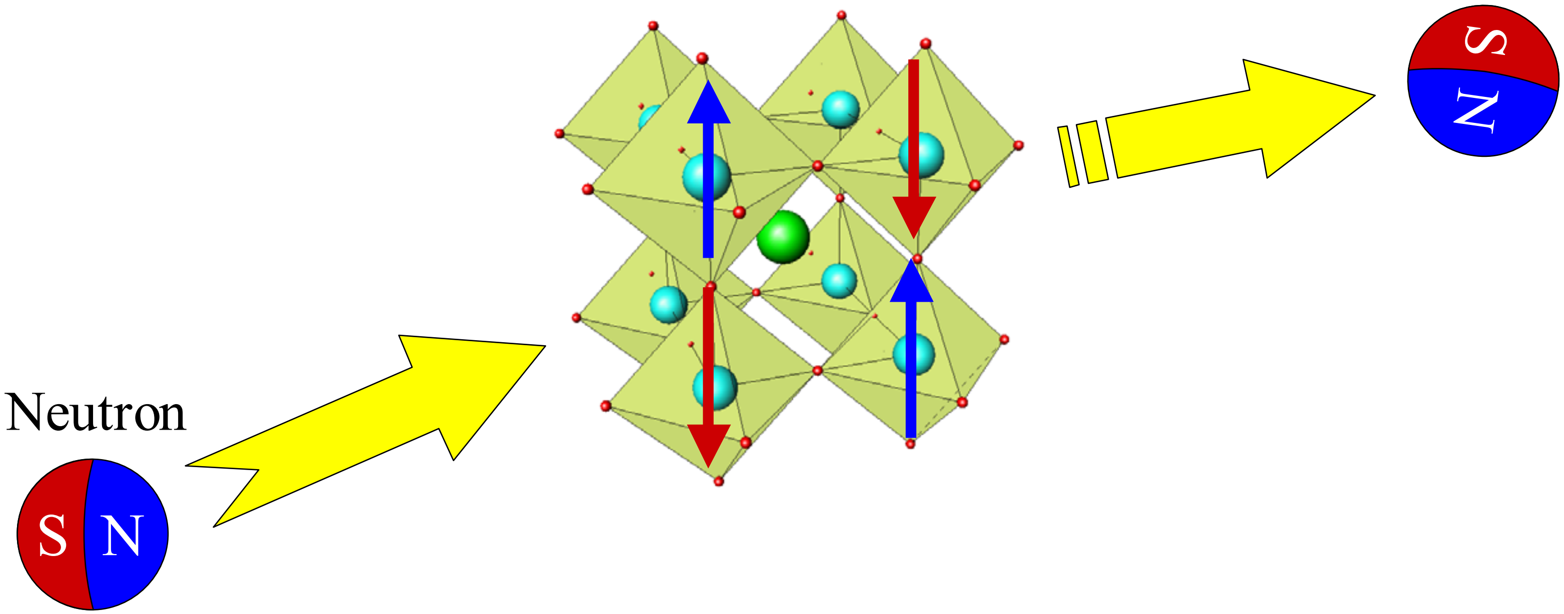
Understanding the ground state

Christian Rüegg PSI/UCL



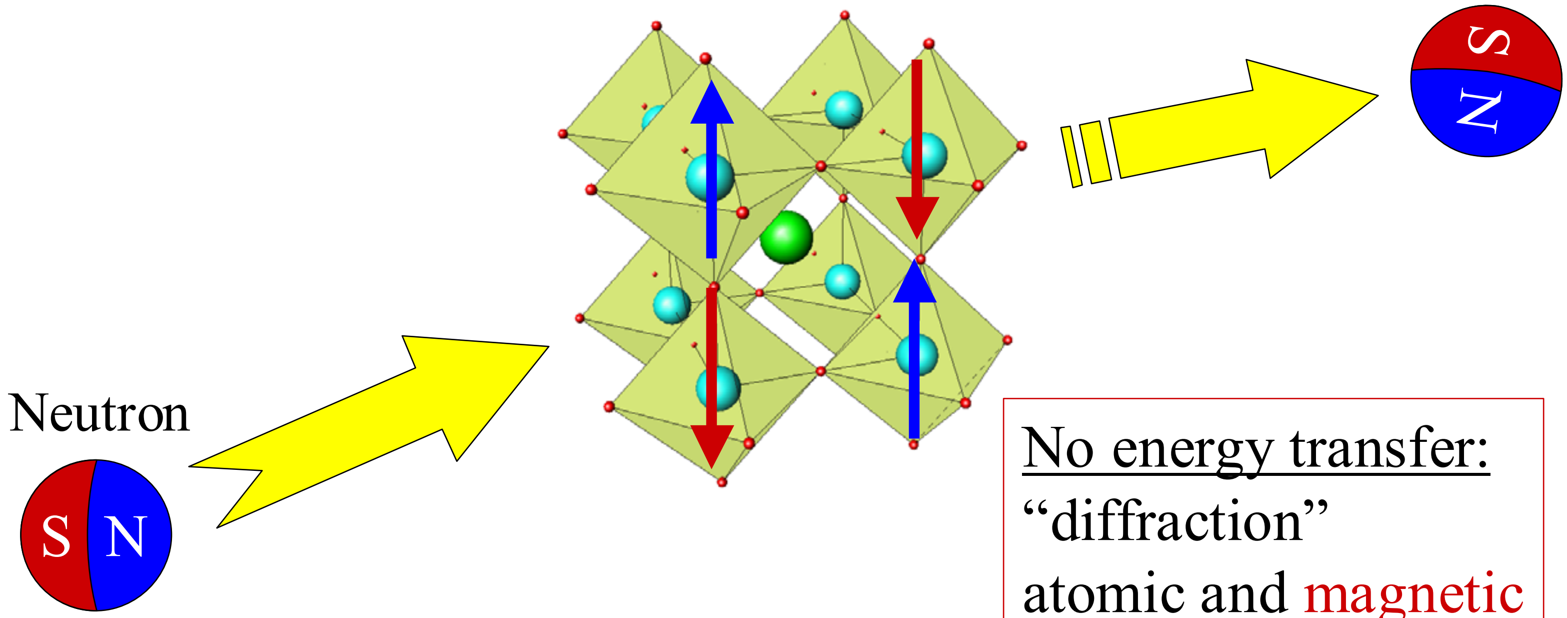
Understanding the ground state

Christian Rüegg PSI/UCL



Understanding the ground state

Christian Rüegg PSI/UCL



No energy transfer:
"diffraction"
atomic and magnetic structure

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Understanding the ground state

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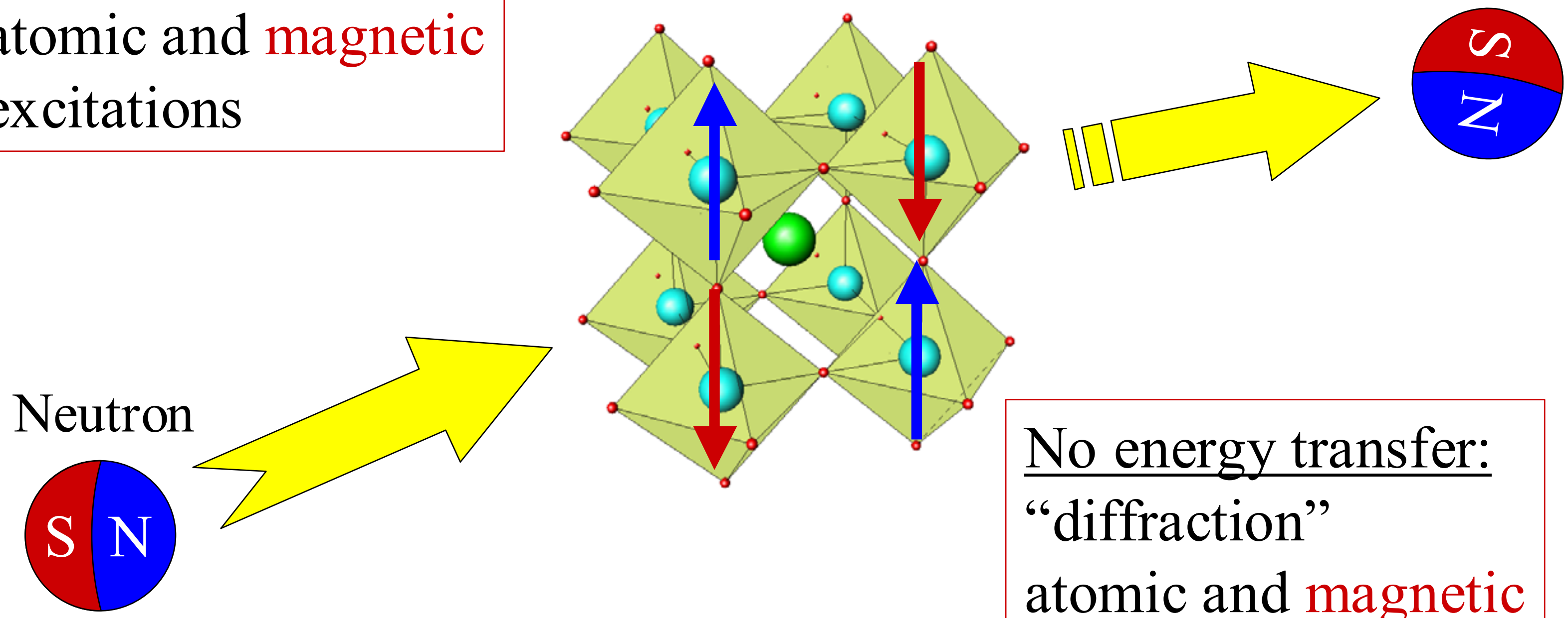
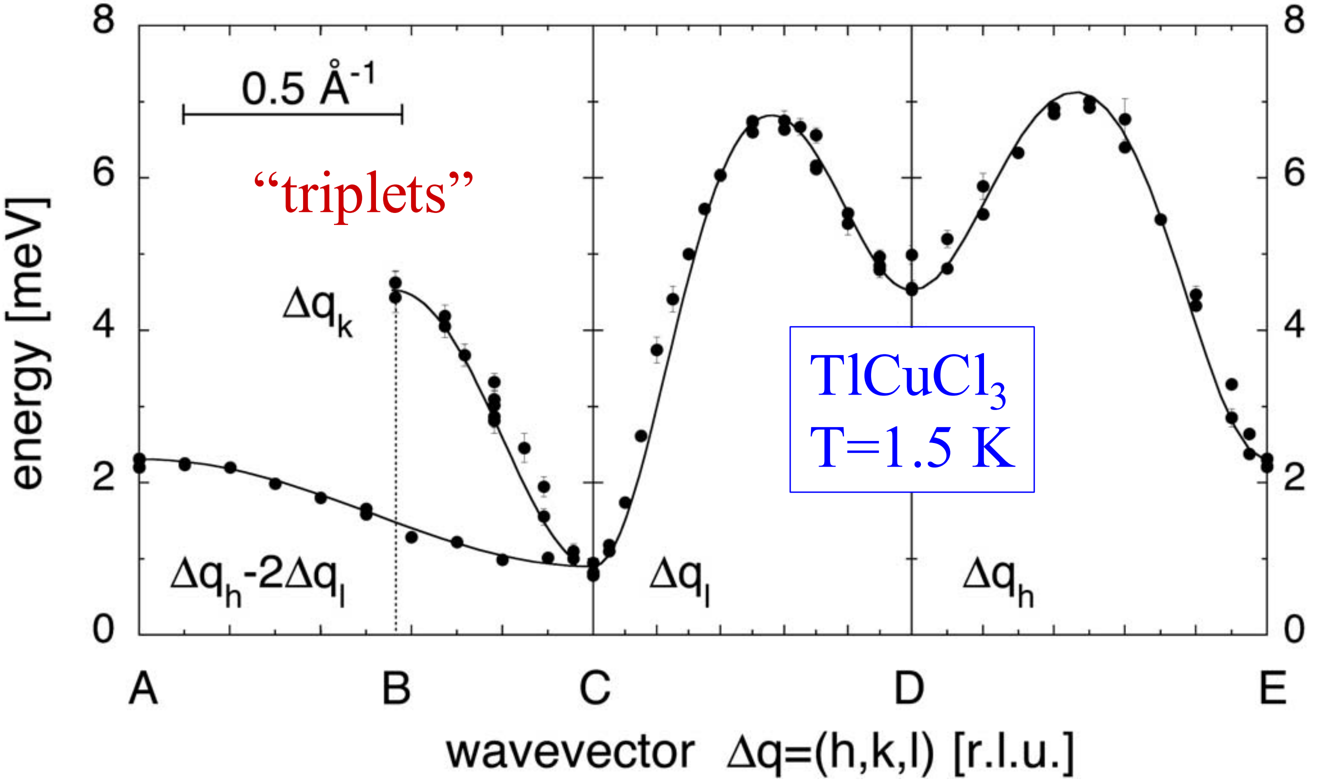
Energy transfer:
"spectroscopy"
atomic and magnetic
excitations



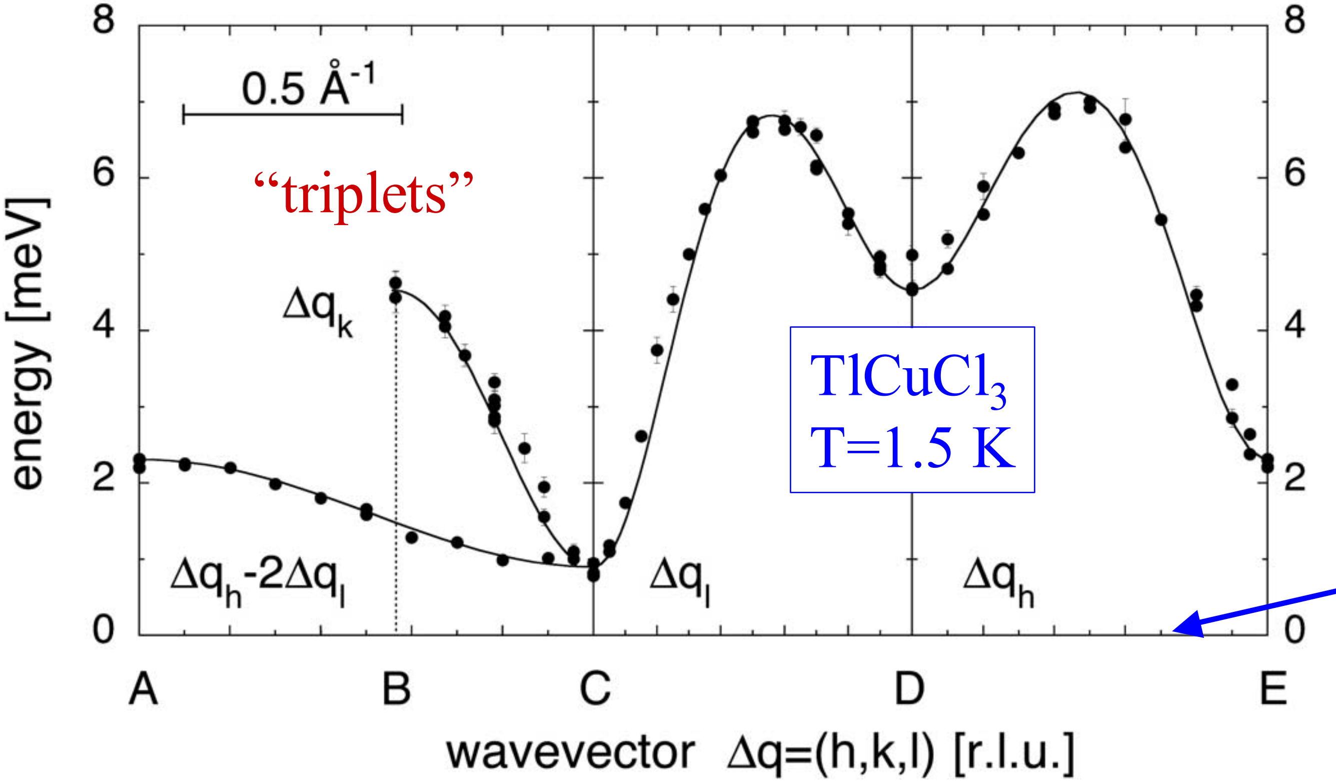
No energy transfer:
"diffraction"
atomic and magnetic
structure

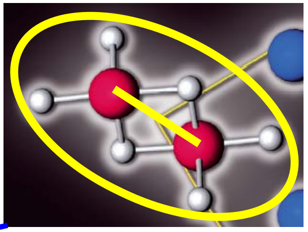
Magnetic excitations



- N. Cavadini et *al.*, Phys. Rev. B **63**, 172414 (2001)
- N. Cavadini et *al.*, J. Phys.: Condens. Matter **12**, 5463 (2000)

Magnetic excitations





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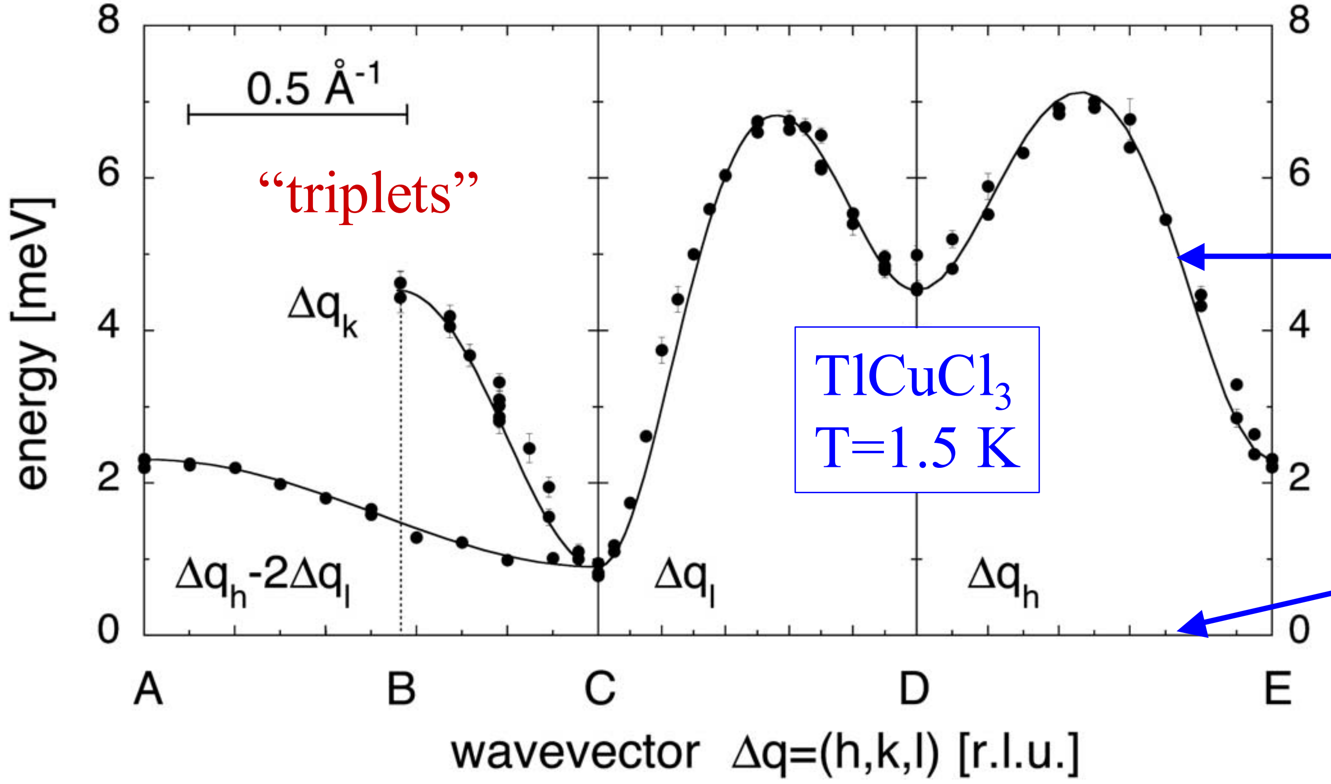
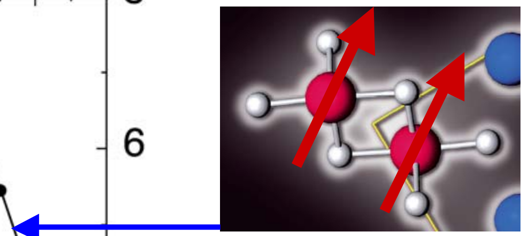
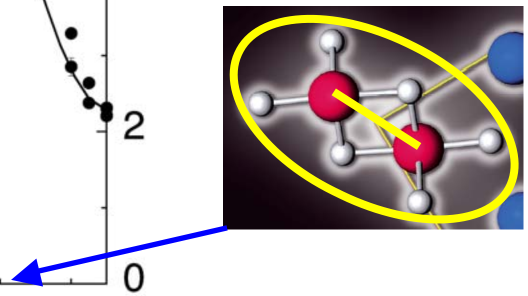
Magnetic excitations







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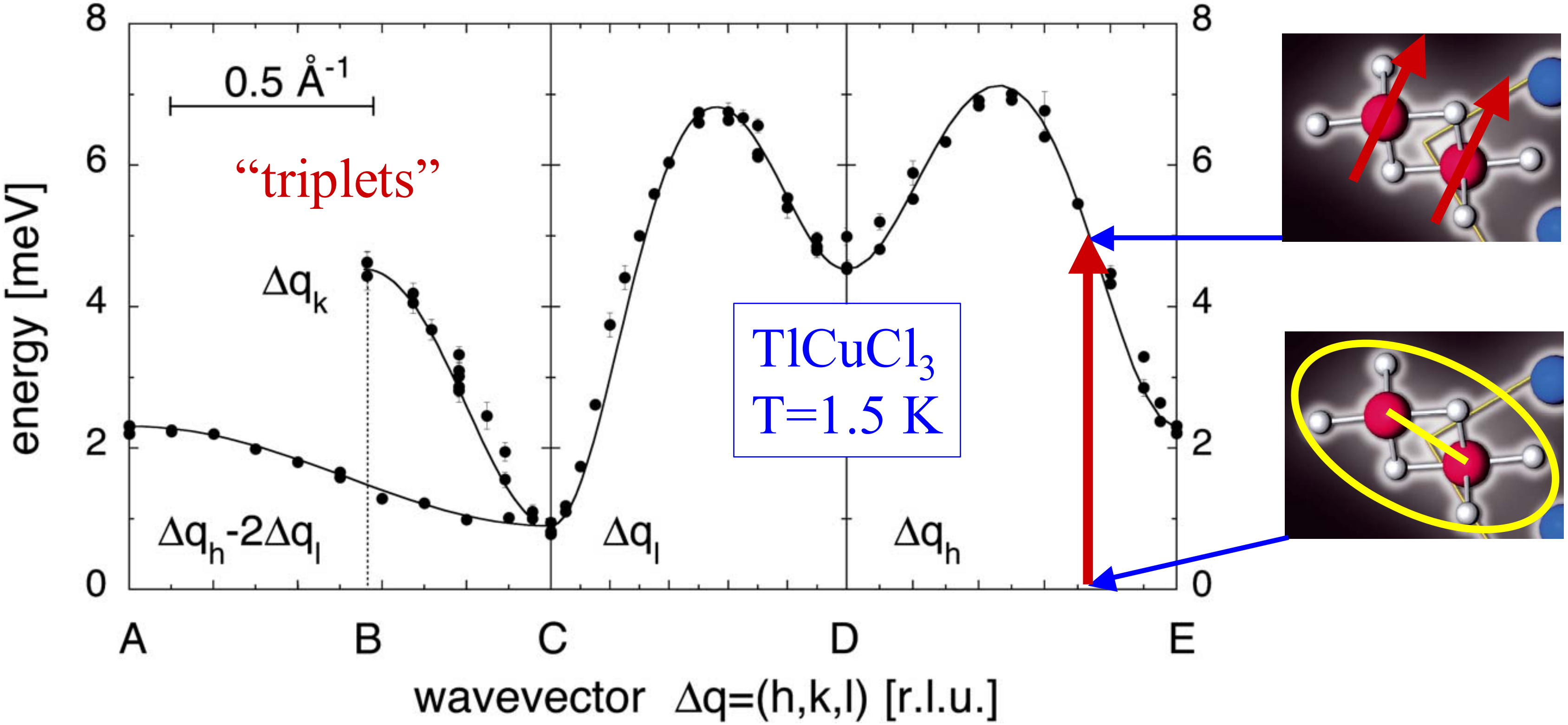
Magnetic excitations



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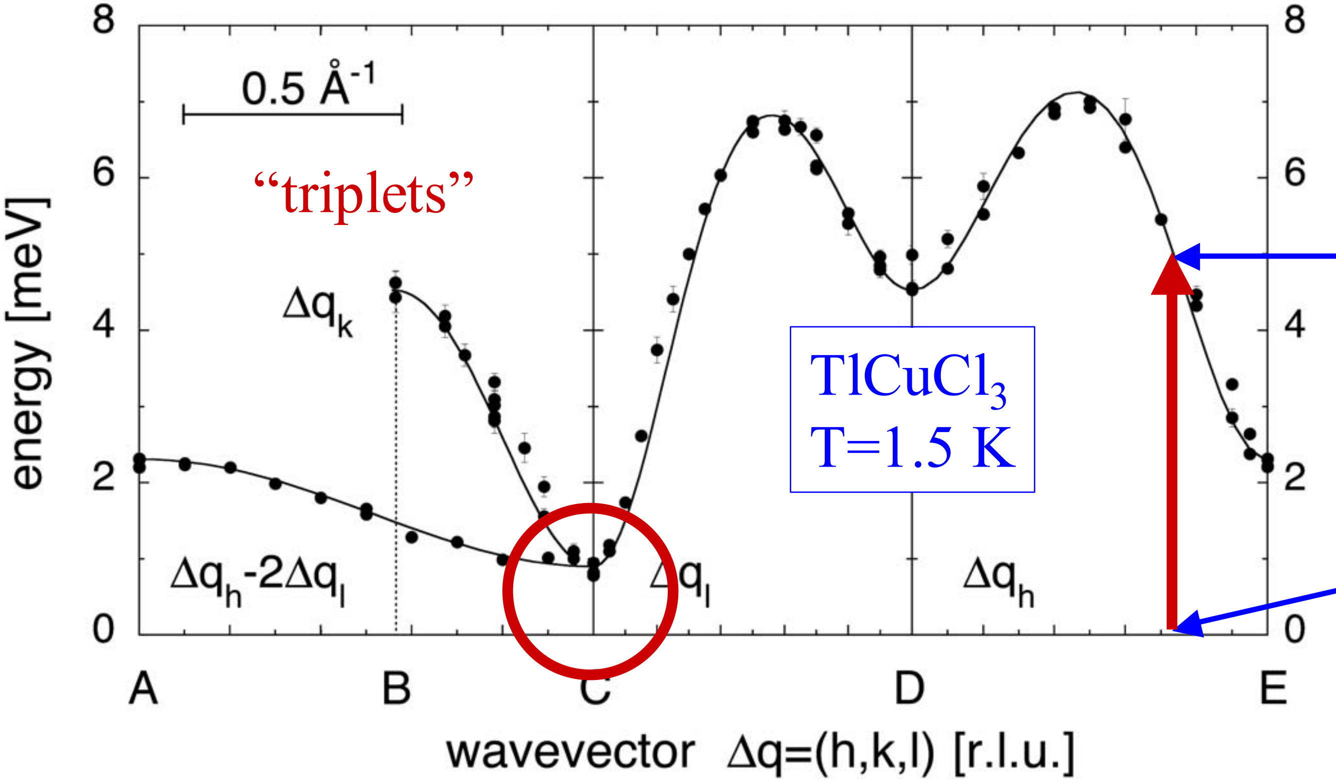
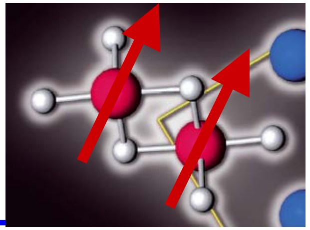
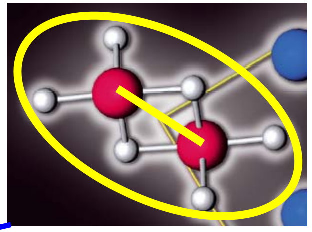
Magnetic excitations







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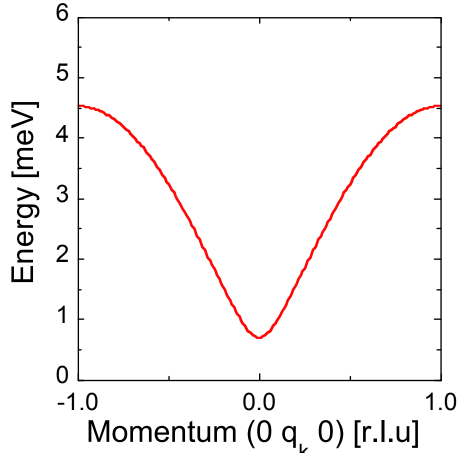
Above the quantumphase transition

SPIN LIQUID



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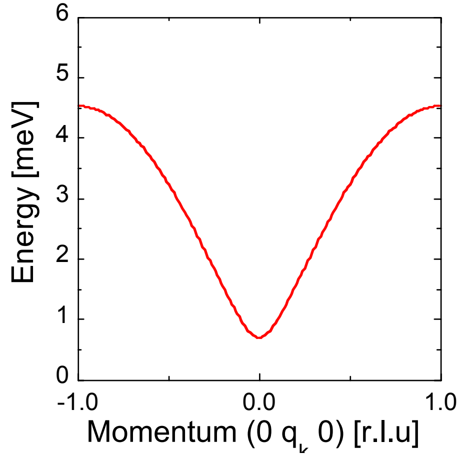
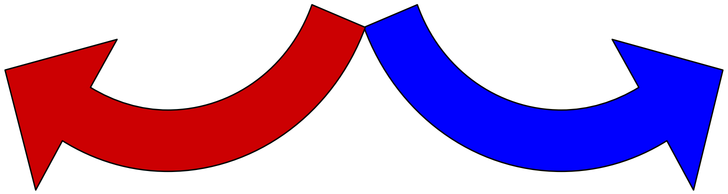
Above the quantumphase transition

SPIN LIQUID



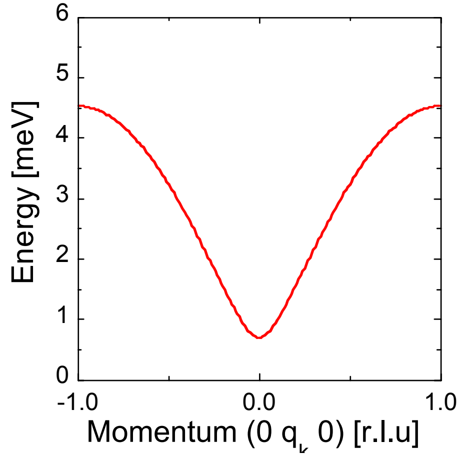


Magnetic field

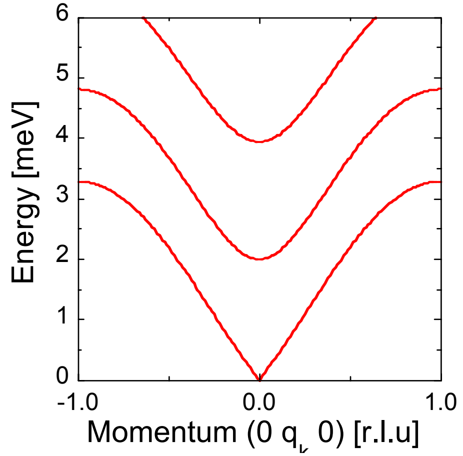
- Ch. Rüegg *et al.*, Nature **423**, 62 (2003)

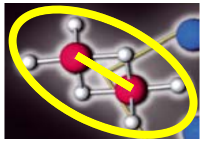
Above the quantumphase transition

SPIN LIQUID



BOSE-EINSTEIN CONDENSATE

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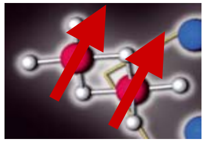
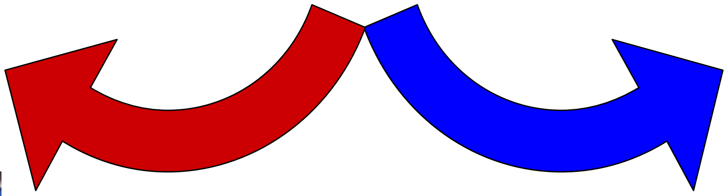


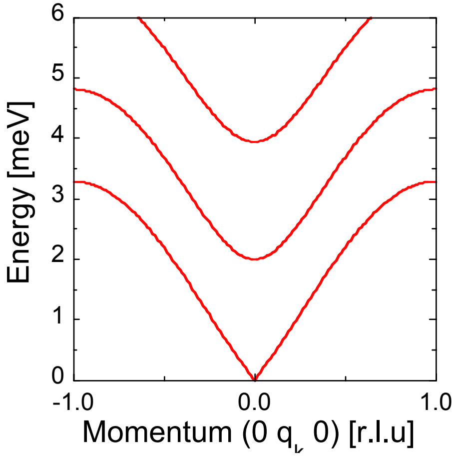


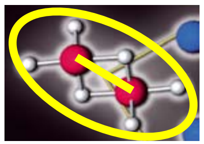
Magnetic field

• Ch. Rüegg *et al.*, Nature **423**, 62 (2003)

Above the quantumphase transition

BOSE-EINSTEIN CONDENSATE

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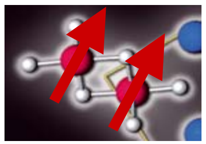

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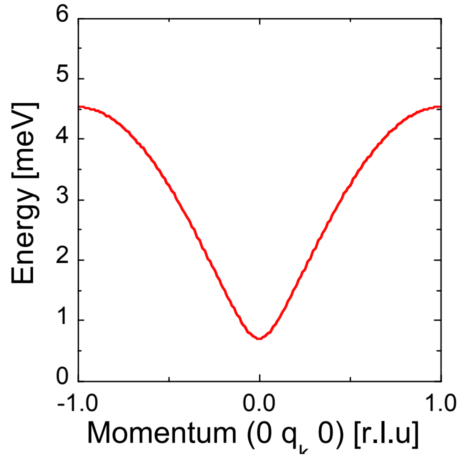
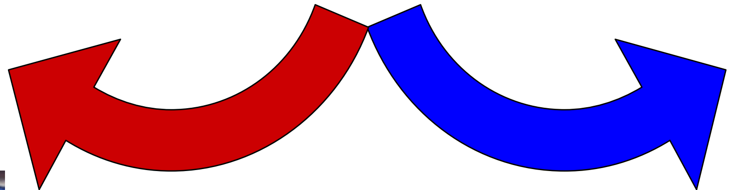
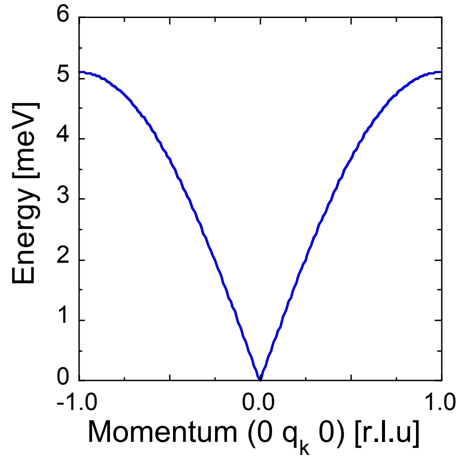
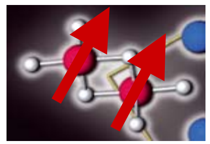




Magnetic field

NEEL STATE

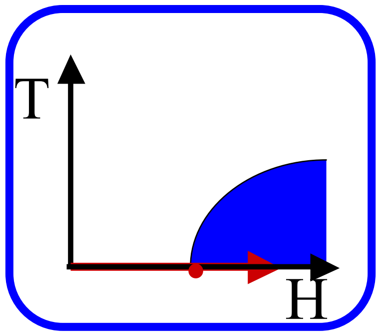


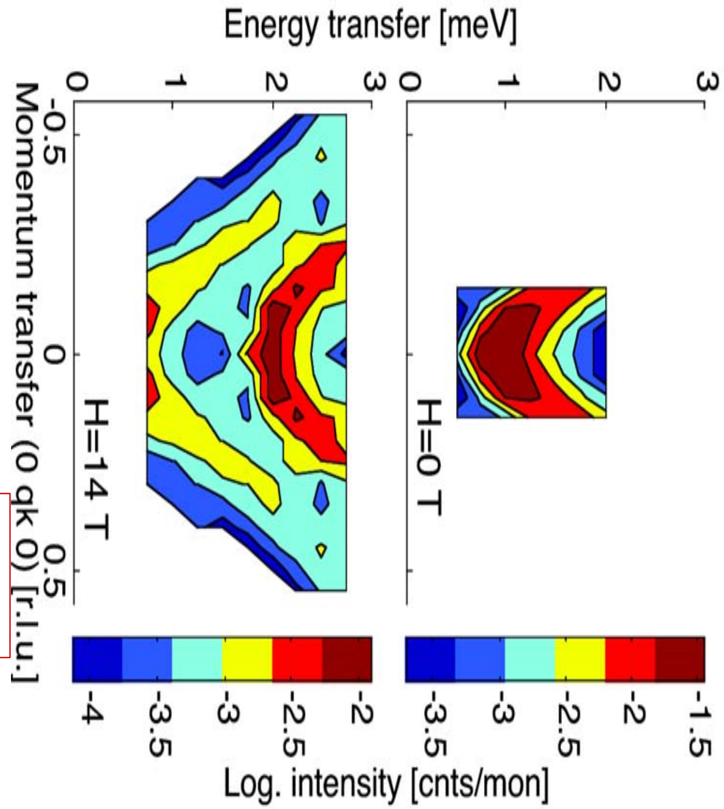


- Ch. Rüegg *et al.*, Nature **423**, 62 (2003)

BOSE-EINSTEIN CONDENSATE

The first time observed in a magnetic system





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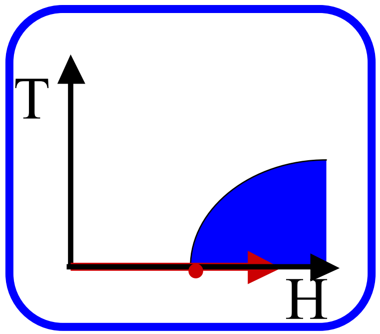

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SPIN LIQUID

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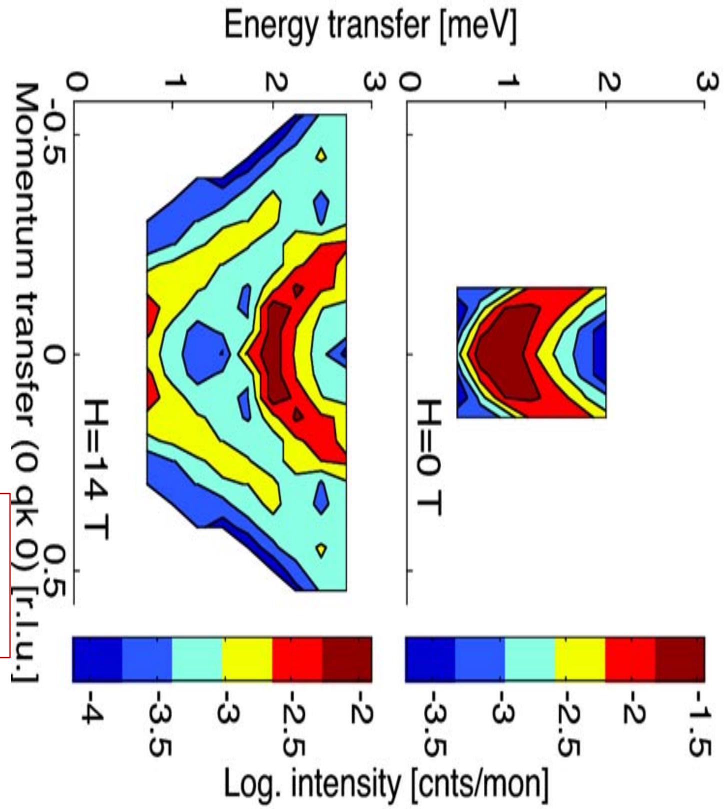

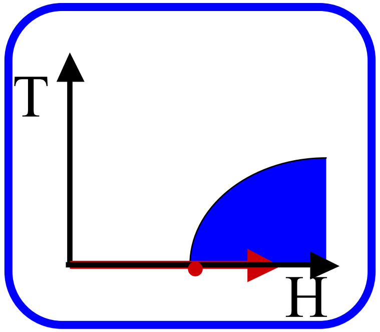

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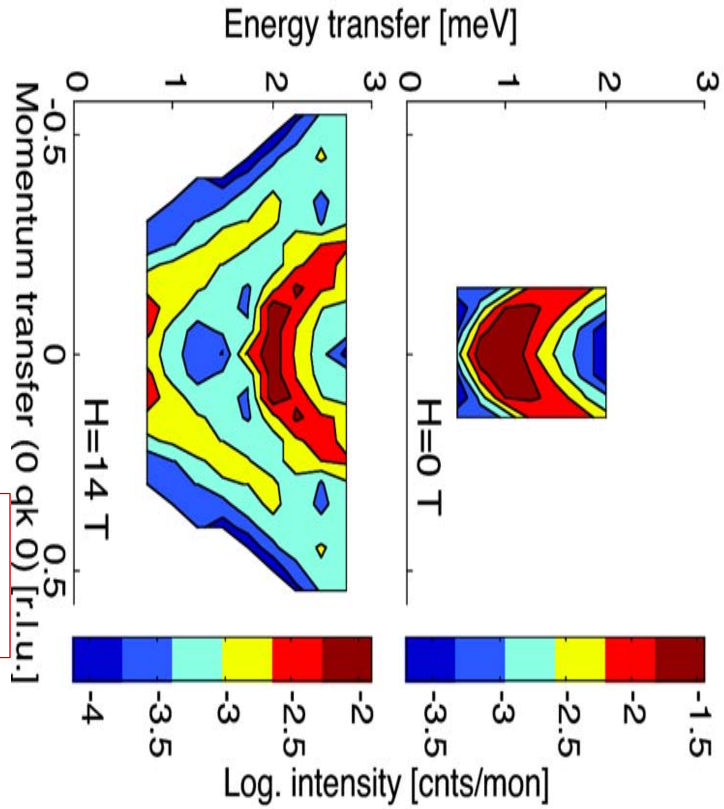

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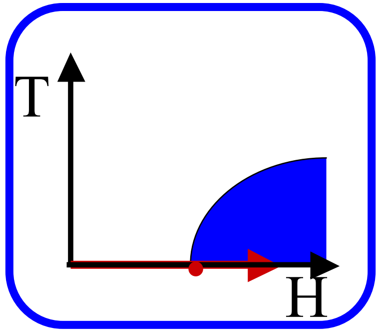
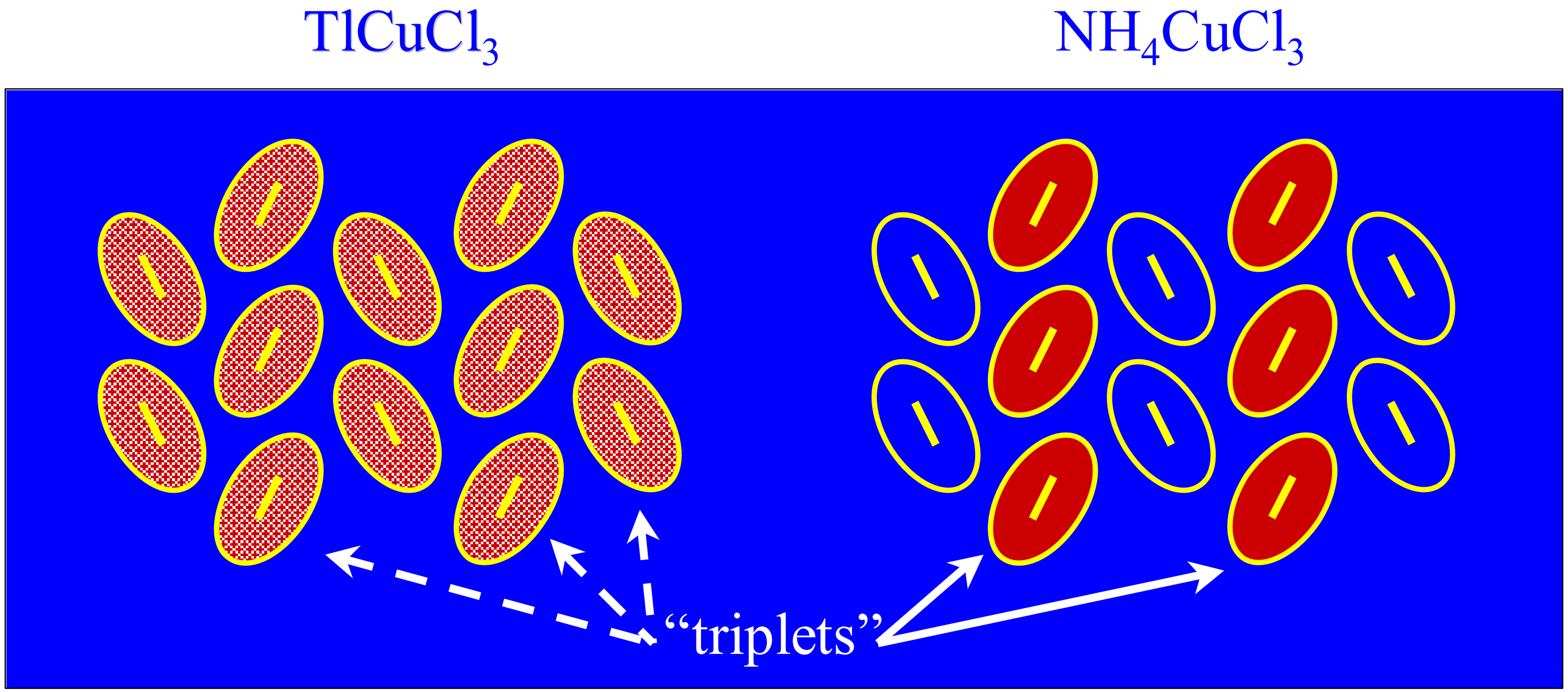
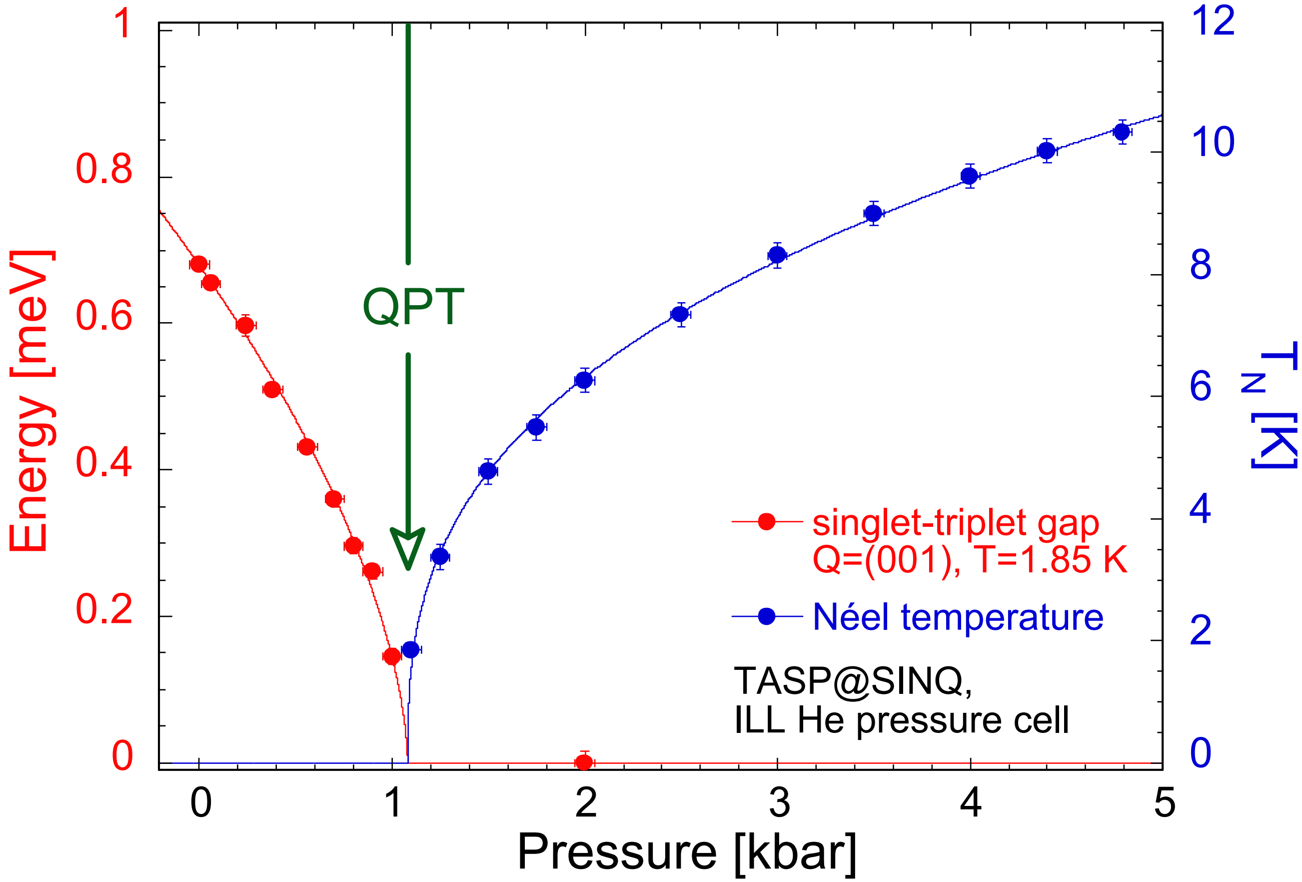




• Ch. Rüegg *et al.*, Nature **423**, 62 (2003)

• Ch. Rüegg *et al.*, Phys. Rev. Lett. **93**, 037207 (2004)

Quantum phase transition with pressure



• Ch. Rüegg *et al.*, submitted to Phys. Rev. Lett.

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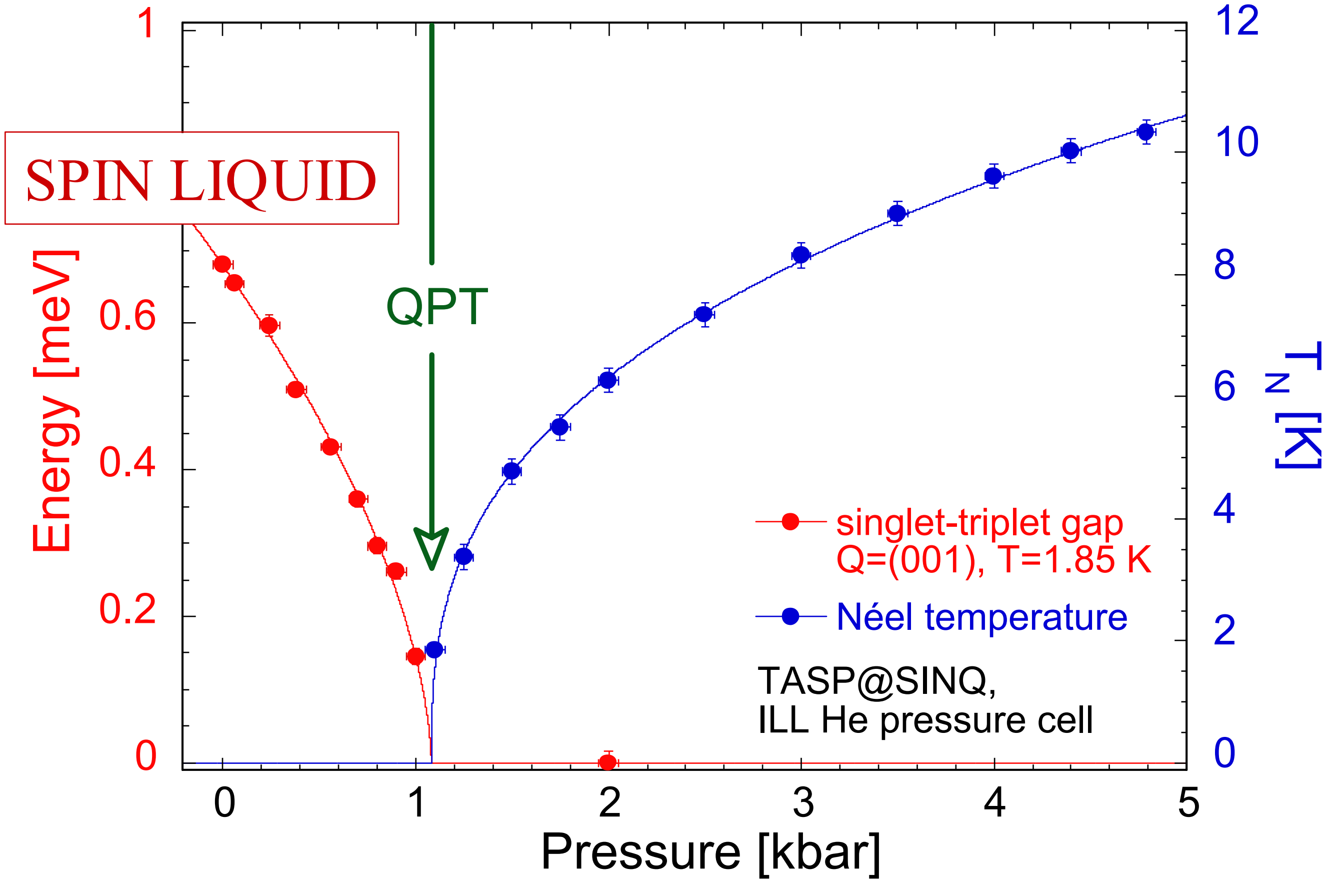
Quantum phase transition with pressure



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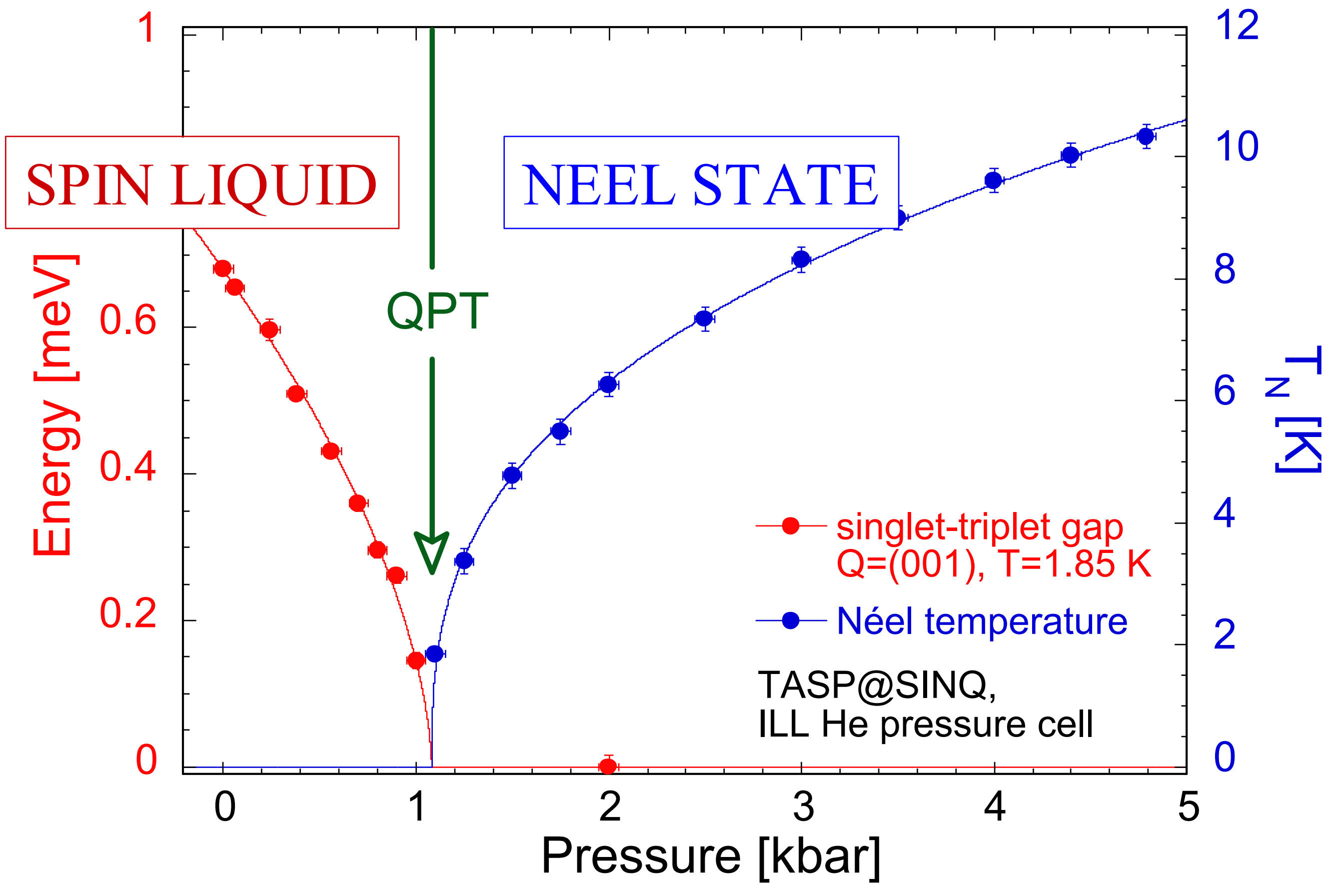
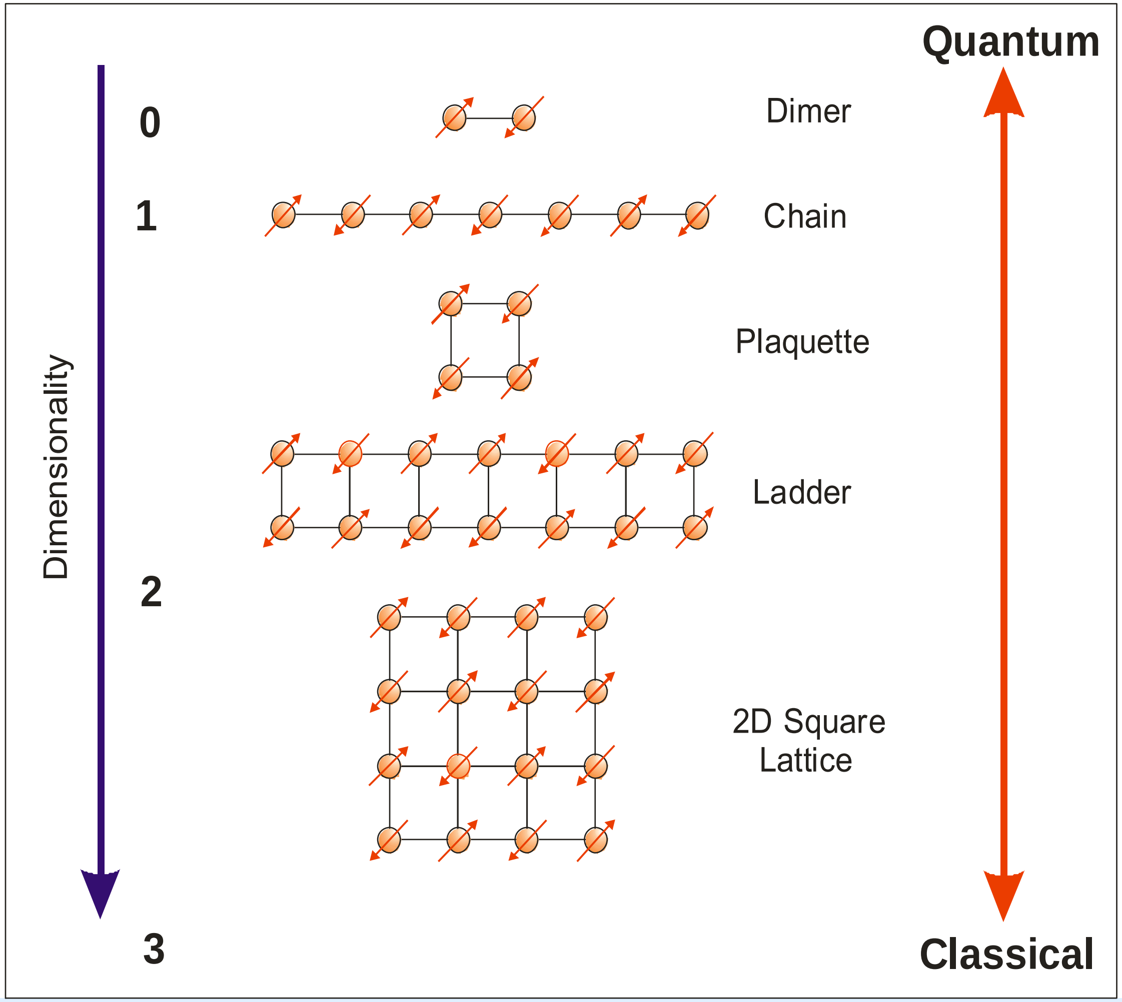


• Ch. Rüegg *et al.*, submitted to Phys. Rev. Lett.

Magnetic Architecture



Two dimensions: border between classical and quantum world

Henrik Rönnow ETH/PSI

Building models

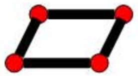
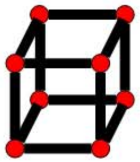
- Spins

  Length: |S|=1/2 … ∞

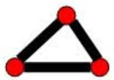
  Quantum / classical

  Dimension: Ising, XY, Heisenberg

- Architecture

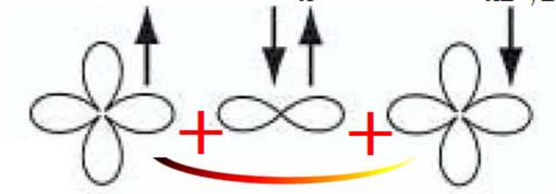




  Dimension

  Connectivity 

- Interactions

  Cu^{2+} O $2p_x$ Cu $3d_{x2-y2}$



  ☞ $= J \sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j$

  Anti-/Ferromagnetic

- Extentions

  Randomness

  Charge, orbit, lattice...

Outlook: Physicist's Lego

H Luetkens PSI

Magnetic properties

P

FM

AFM

CMR

MF

Electric properties

M | I

FE | SC

AFE

Combinations

Fundamental Science

- Competition of ground states
- Coexistence of ground states
- Coupling of different ground states
- (Giant) proximity effects
- Electric field effects (2D-electron gas, ...)
- …

Applications

- Spintronics (Switching of currents with magnetic fields)
- Sensors (Magnetism, pressure, temperature, gases, …)
- Actuators
- Non-volatile memory (MRAM, …)
- …

Outlook: Physicist's Lego

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Applications

- Spintronics (Switching of currents with magnetic fields)
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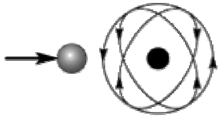
- Actuators
- Non-volatile memory (MRAM, …)
- …

IT and quantum devices

- Giant magnetoresistance and exchange bias for spintronics and high density data storage
- Hard thin film magnets for micro-motors, -switches and -sensors
- Understanding magnetic roughness and phase diagrams - towards better electronic devices
- Understanding quantum complexity

Uniqueness of Neutrons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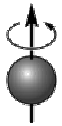
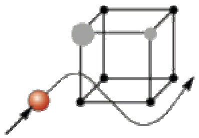
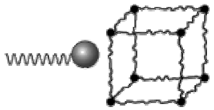
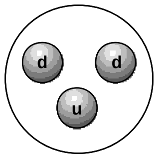

2. Neutrons see Elementary Magnets


3. **Neutrons see Light Atoms next to Heavy Ones**


4. Neutrons measure the Velocity of Atoms

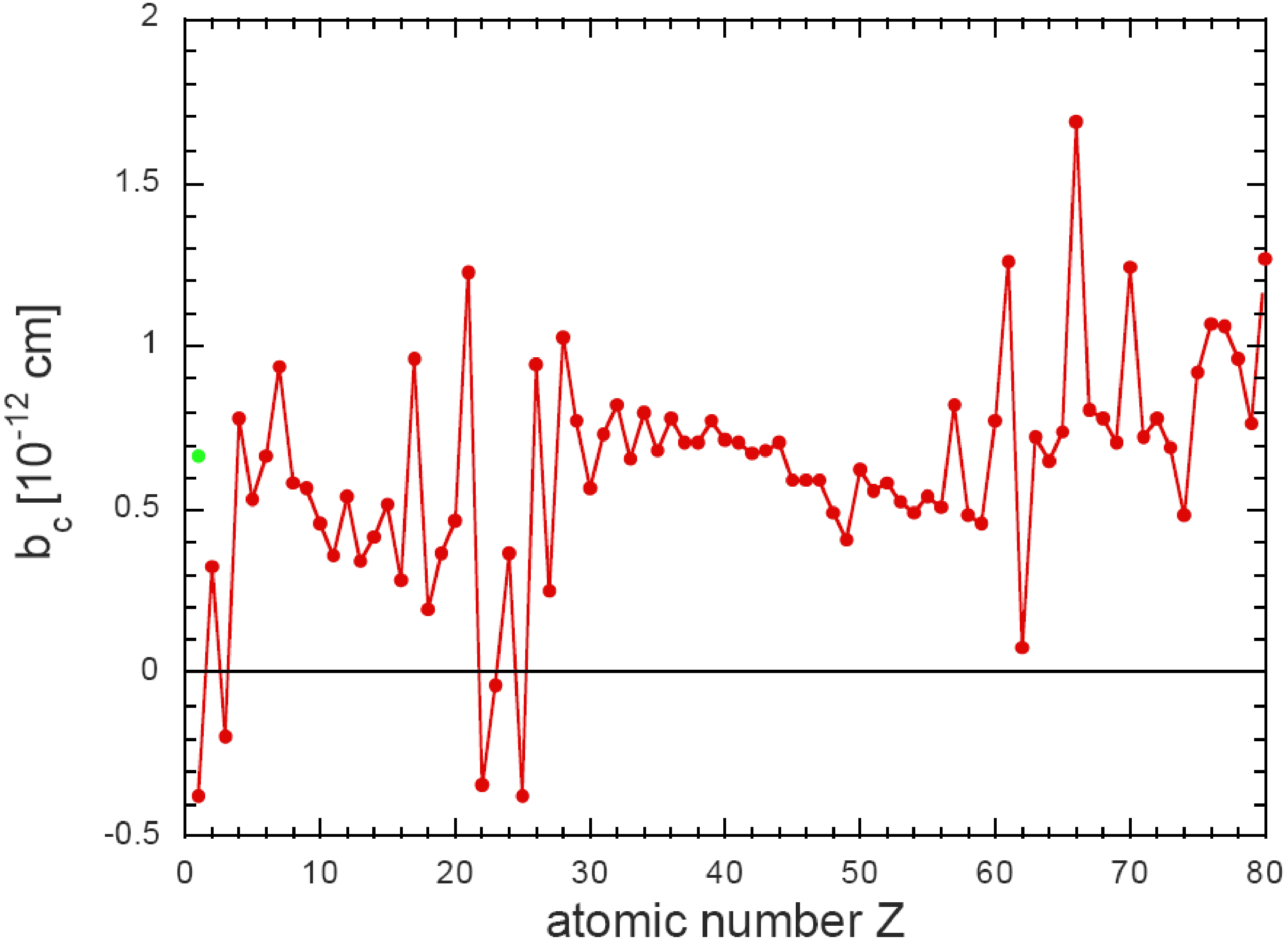

5. Neutrons penetrate deep into Matter



6. Neutrons are Elementary Particles

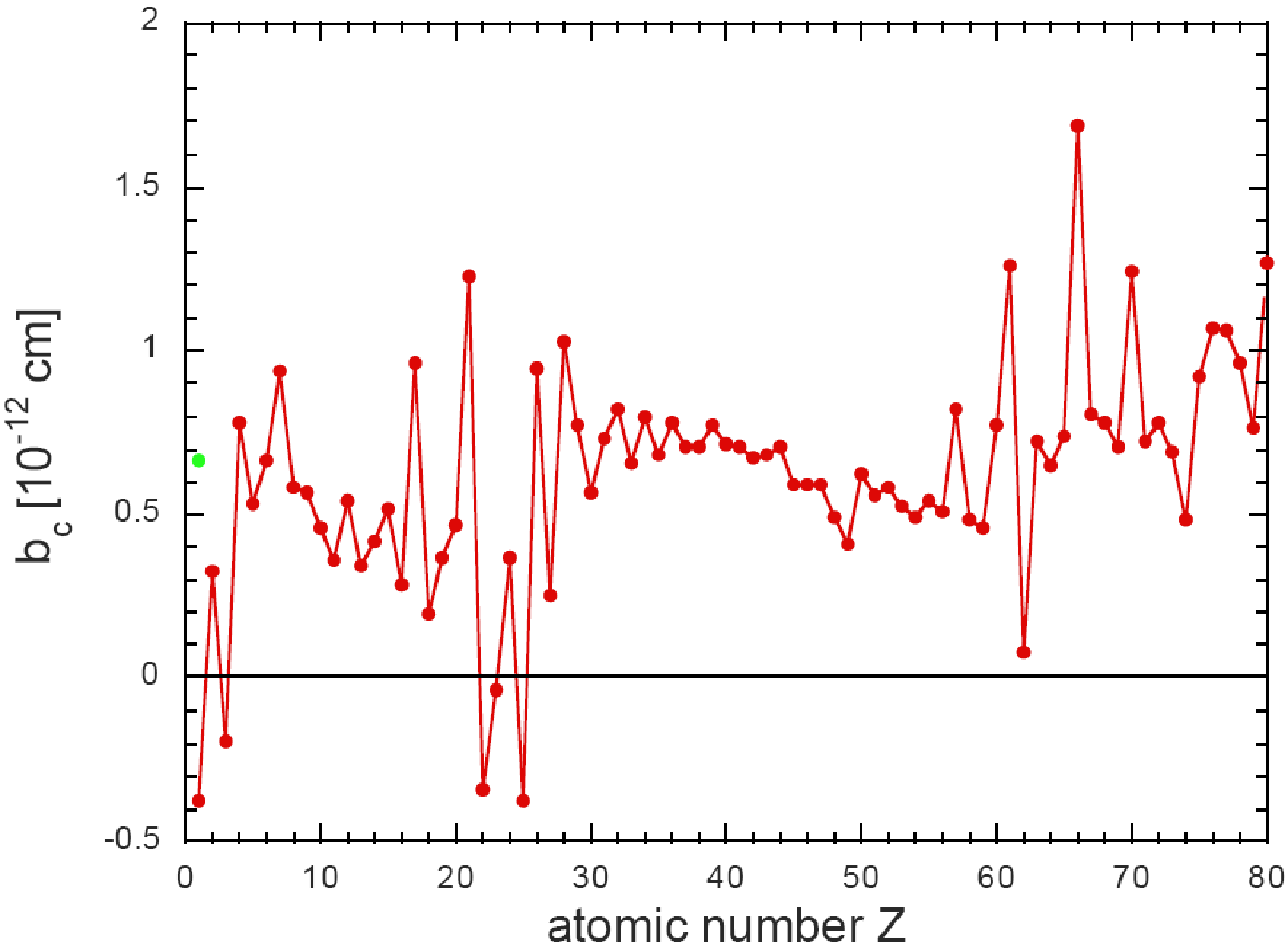
PAUL SCHERRER INSTITUT PSI

Coherent Neutron Scattering Length [fm]



Scattered Intensity proportional to b^2

Coherent Neutron Scattering Length [fm]



Scattered Intensity proportional to b^2

For X-rays:

b α Z

I α Z^2

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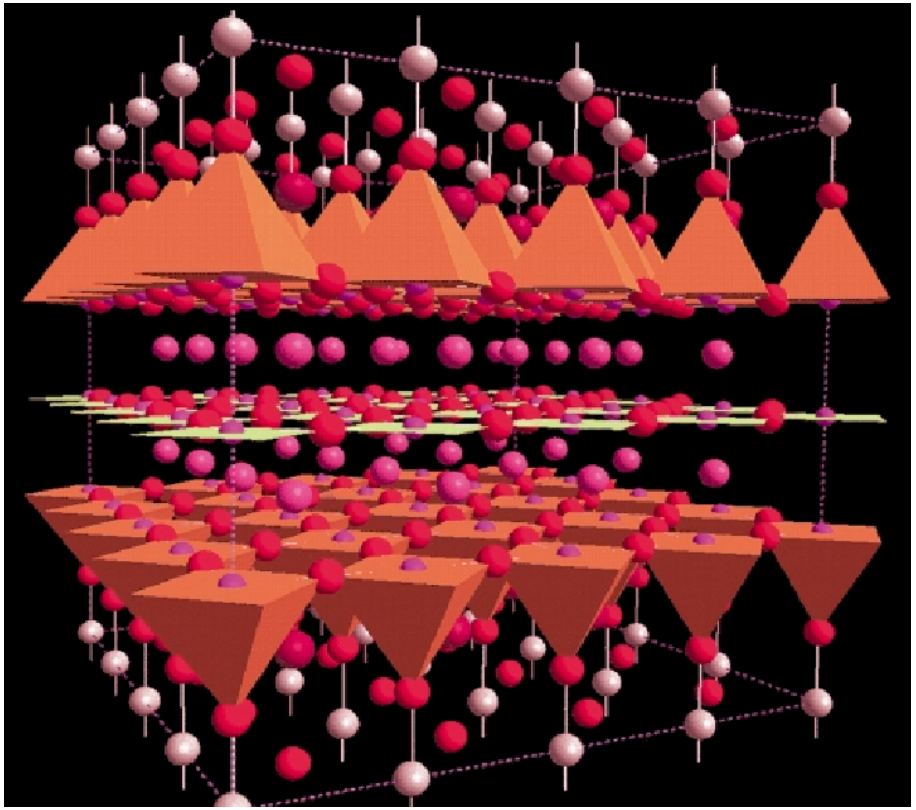
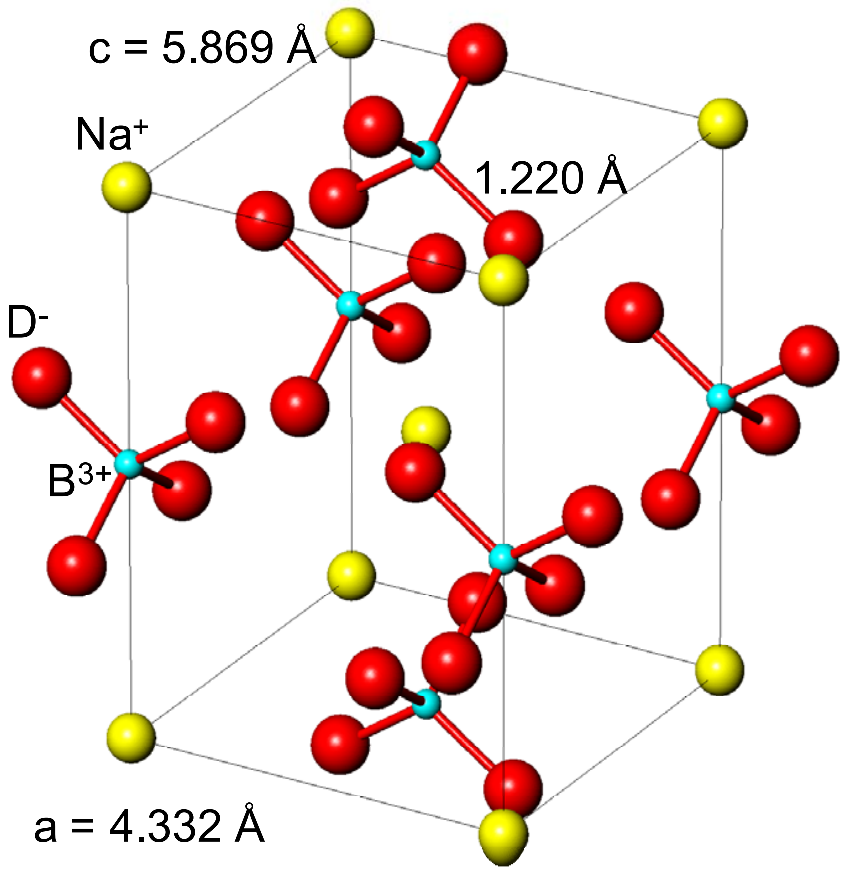
Neutrons see Light Atoms next to Heavy Ones



Crucial oxygen positions revealed by neutrons

High temperature superconductors for the technology of tomorrow.

Order-Disorder phase transition due to reorientation of BD_4^- tetrahedra in **$NaBD_4$**



V. Pomjakushin PSI

P.Fischer, A. Züttel (2004)

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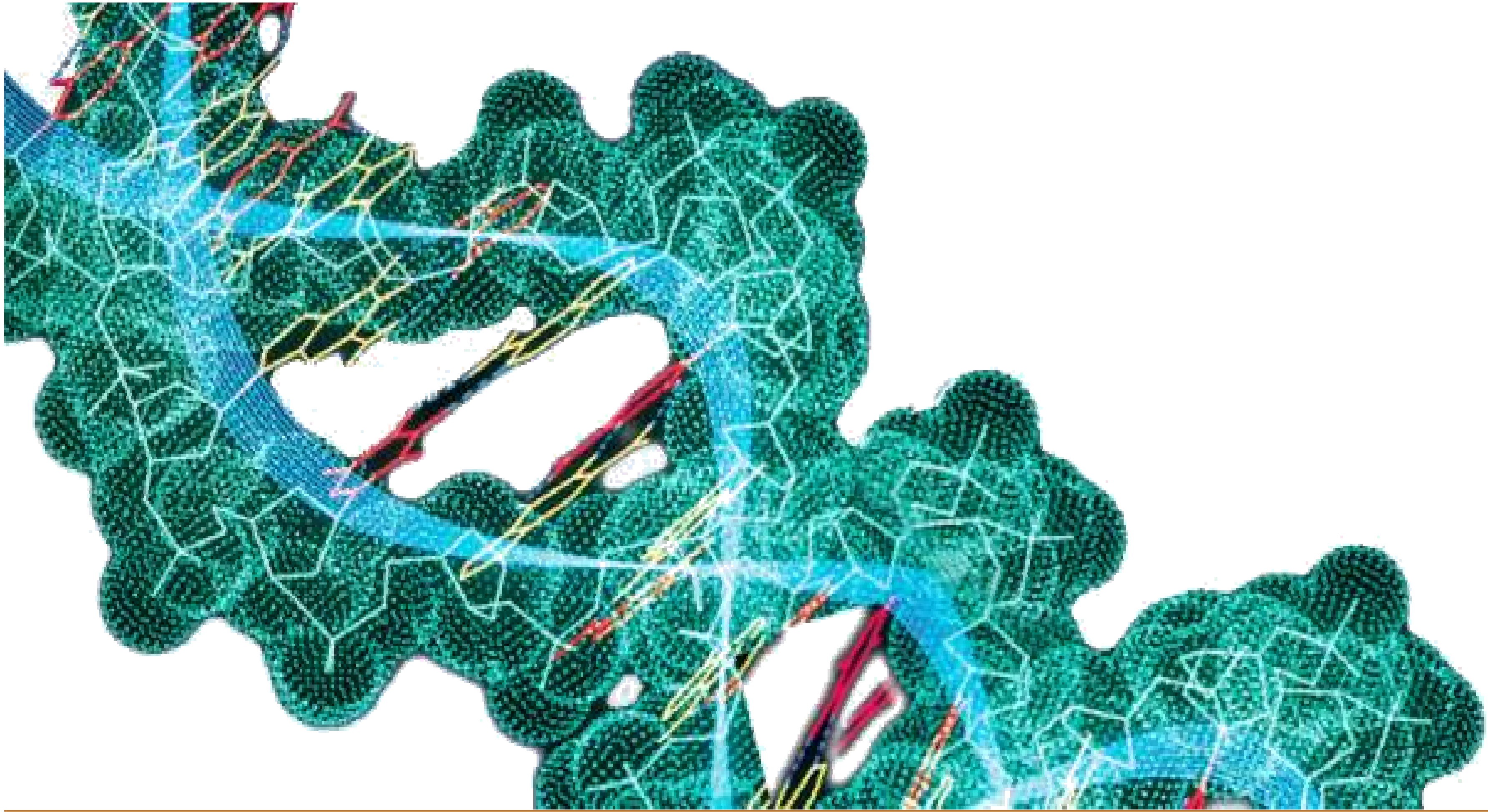
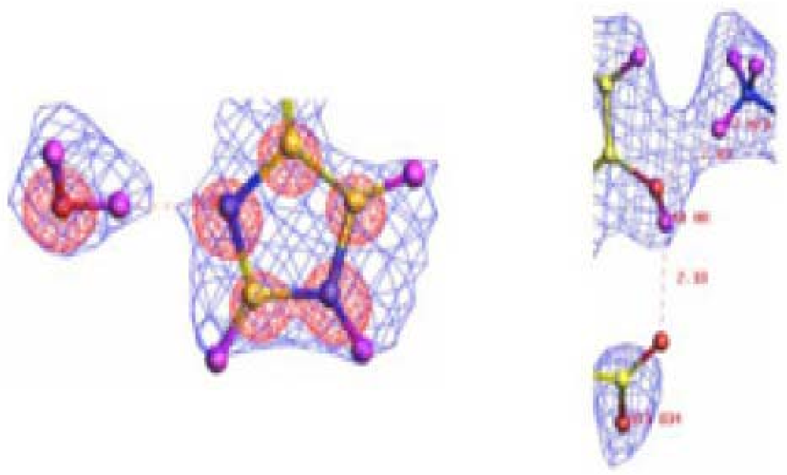
Neutrons see Light Atoms next to Heavy Ones

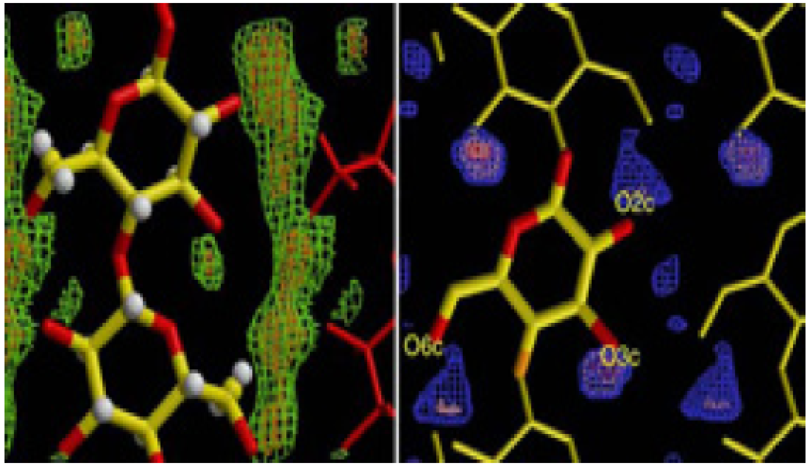


Only neutrons see H-bonds and catalytic H positions.

Locating Hydrogen



Density maps showing the positions of hydrogen atoms in protein crystals as determined by neutron crystallography

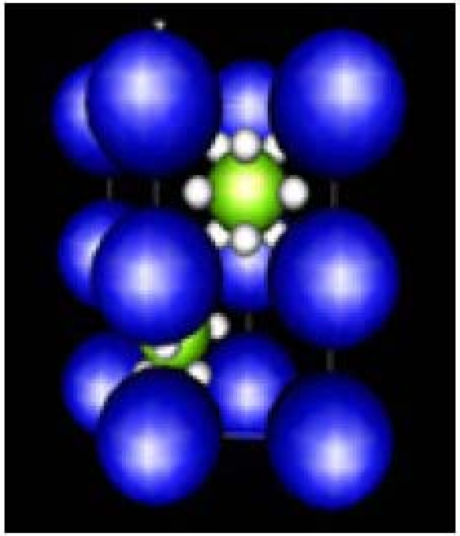


Density maps from neutron high-angle fibre diffraction reveal the hydrogen bonding network in cellulose.

Hydrogen storage materials and batteries

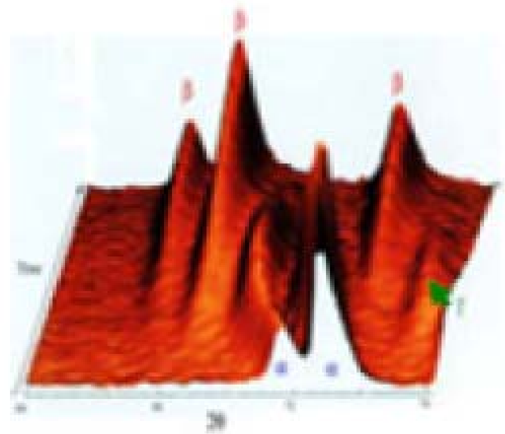
Energy for the future

- Hydrogen storage materials.
- Fuel cell components; oxide ion conductors.
- Clathrate hydrates for energy sources.
- Light, high energy density batteries.
- Energy efficient transport; superalloys, ceramics, fuel additives.



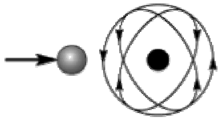
The crystal structure of Mg_2FeH_6

In situ studies of functioning H storage or Battery.

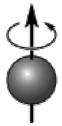


In-situ neutron diffraction during charging of a Ni-MH battery

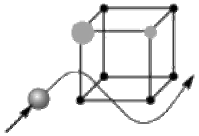
Uniqueness of Neutrons



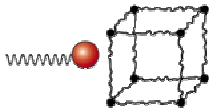
1. Neutrons see the Nuclei



2. Neutrons see Elementary Magnets

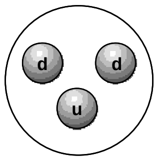


3. Neutrons see Light Atoms next to Heavy Ones



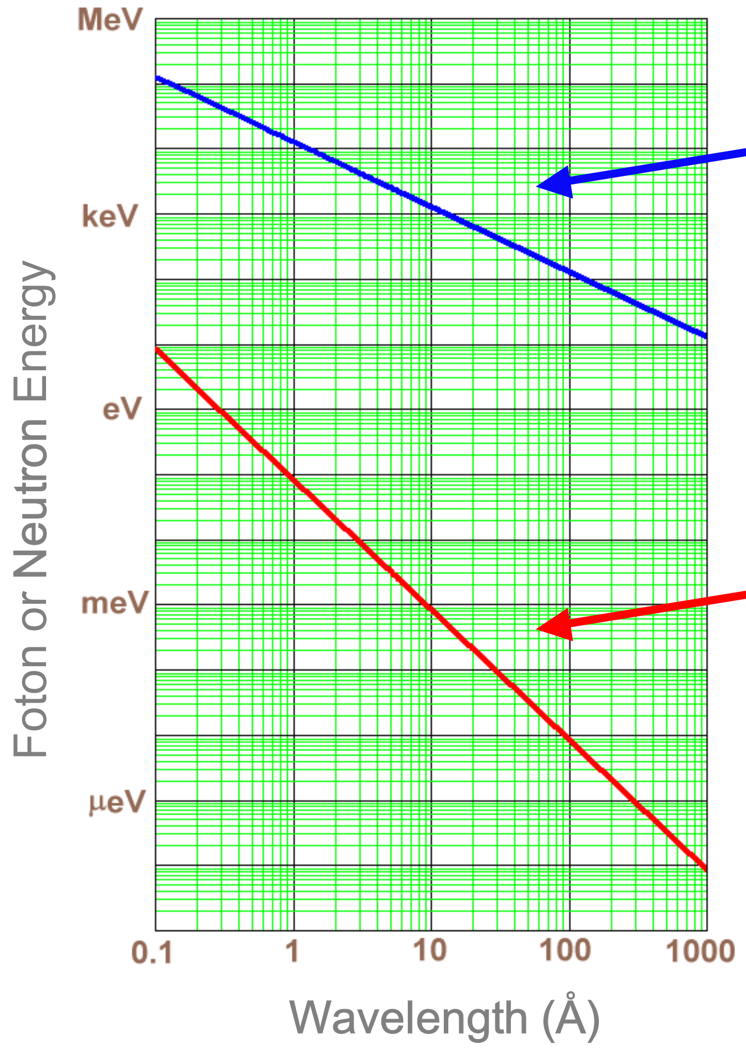
4. Neutrons measure the Velocity of Atoms

5. Neutrons penetrate deep into Matter



6. Neutrons are Elementary Particles

λ ~ d and E ~ exitation Energies in Cond. matter



Fotons:

$(h \cdot \nu)$

$$E = \frac{h \cdot c}{\lambda}$$

Neutrons:

m = 1.67 10^{-27} kg ~ m_{proton}

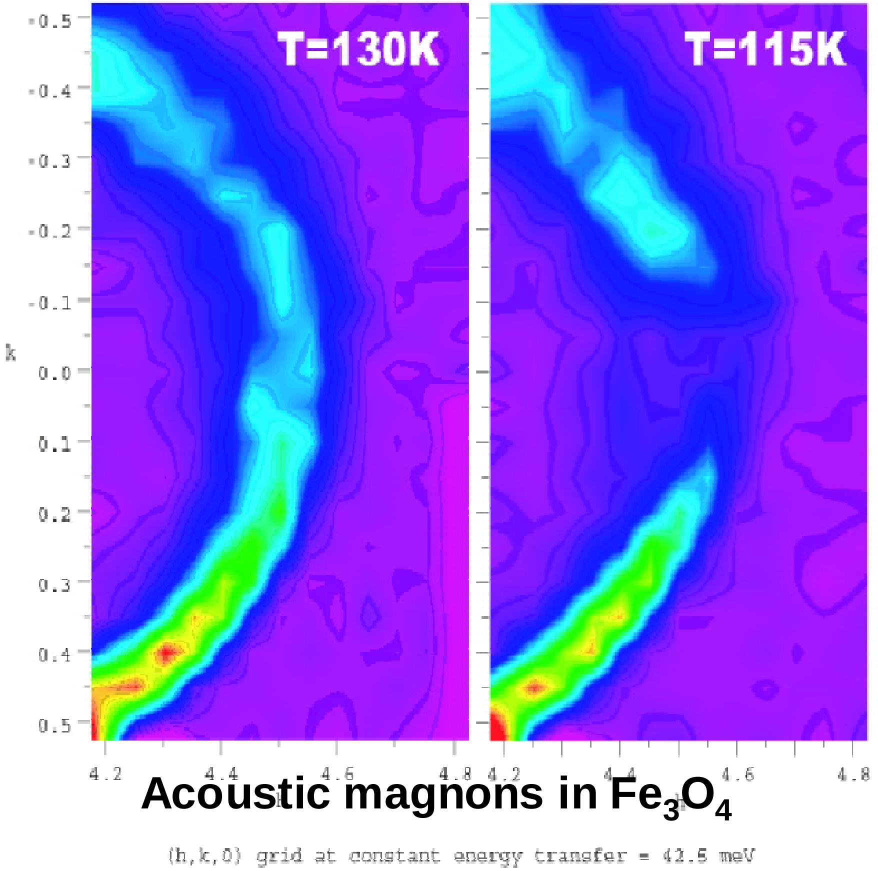
Spin = ½

Charge = 0

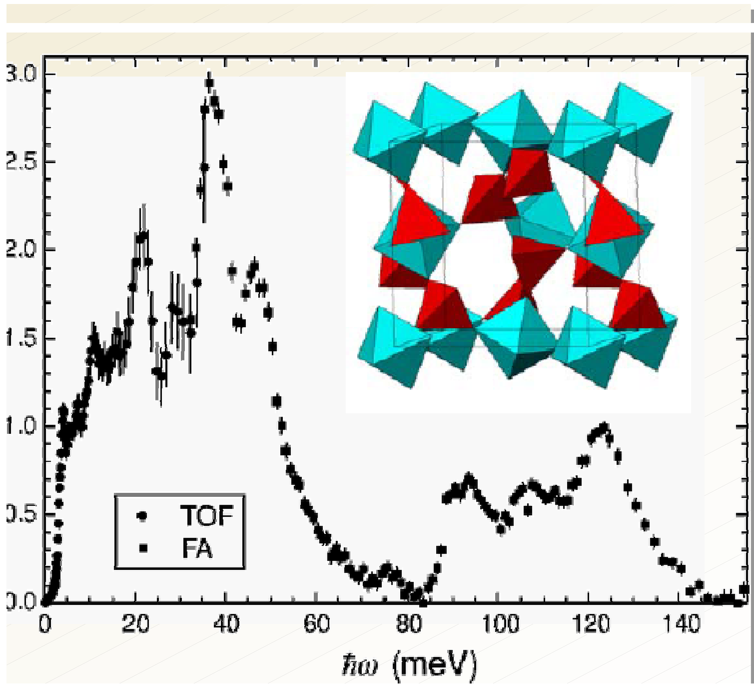
$$E = \frac{h^2}{2 \cdot m \cdot \lambda^2}$$

$(\frac{1}{2} \cdot m \cdot v^2)$

Inelastic scattering



Acoustic magnons in Fe_3O_4



onon density of states of ZrW_2O_8

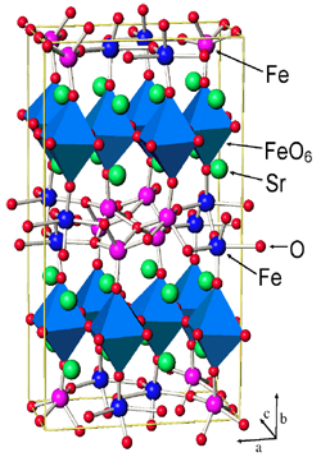
T Mason, SNS

Ionic Conducting Materials: SOFCs, Ceramic Membranes

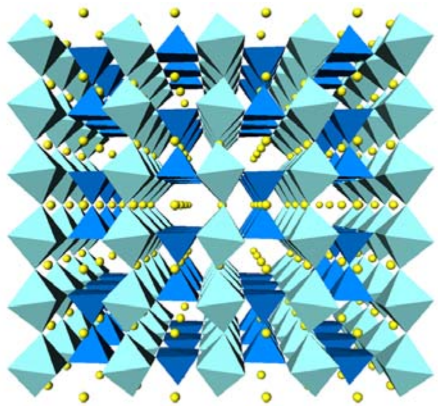
Rietveld Analysis:
performance relationship to composition, crystal structure, phase transitions (order-disorder), microstrain, texture, …

Max-Entropy Analysis:
real space imaging of proton and oxide-ion conducting pathways,

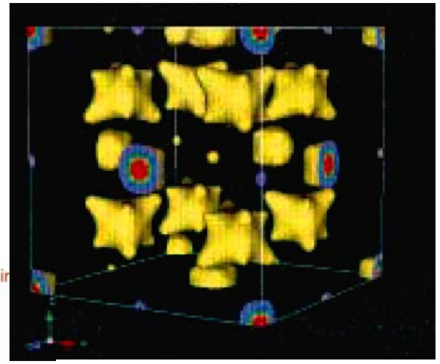
High-Temperature Furnace with Automated Gas Flow Controllers:
dynamic in-situ experiments under realistic conditions (extreme ΔpO_2 and ice formation expts)



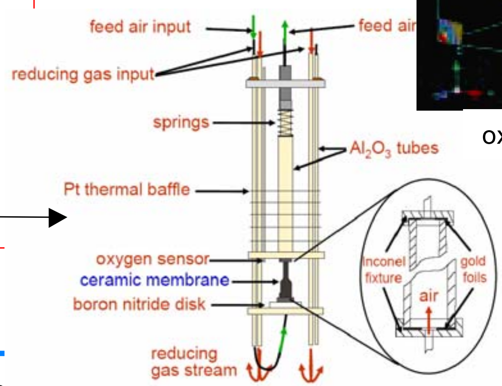
$Sr_2(Fe_{1-x}Co_x)_3O_{6+\delta}$ ↔



$Sr_4(Fe_{1-y}Co_y)_4O_{12}$

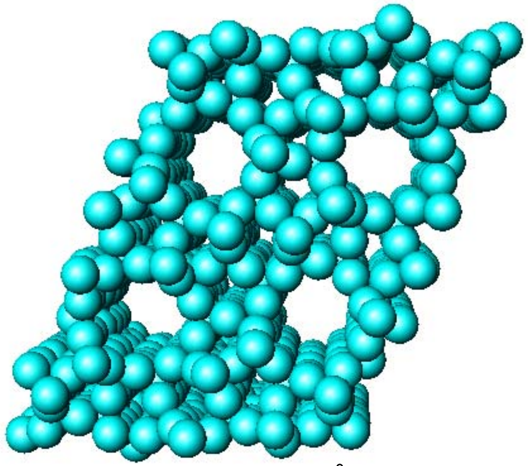


oxide-ion migration in CeO_2 (1497°C)
Appl. Phys. Lett., Vol. 84, No. 4, 26

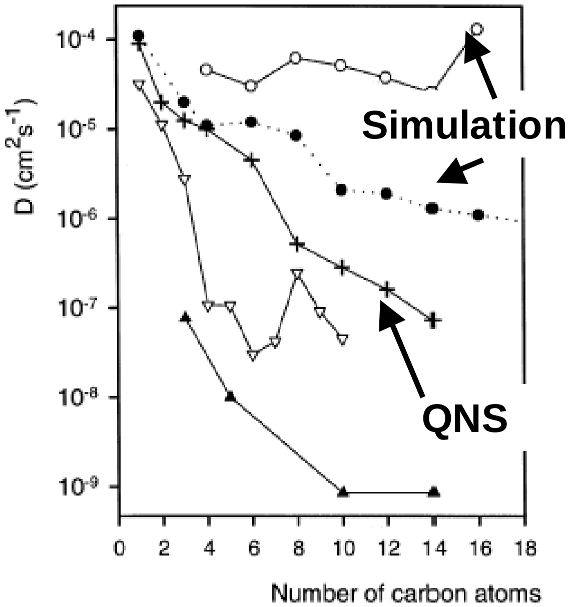


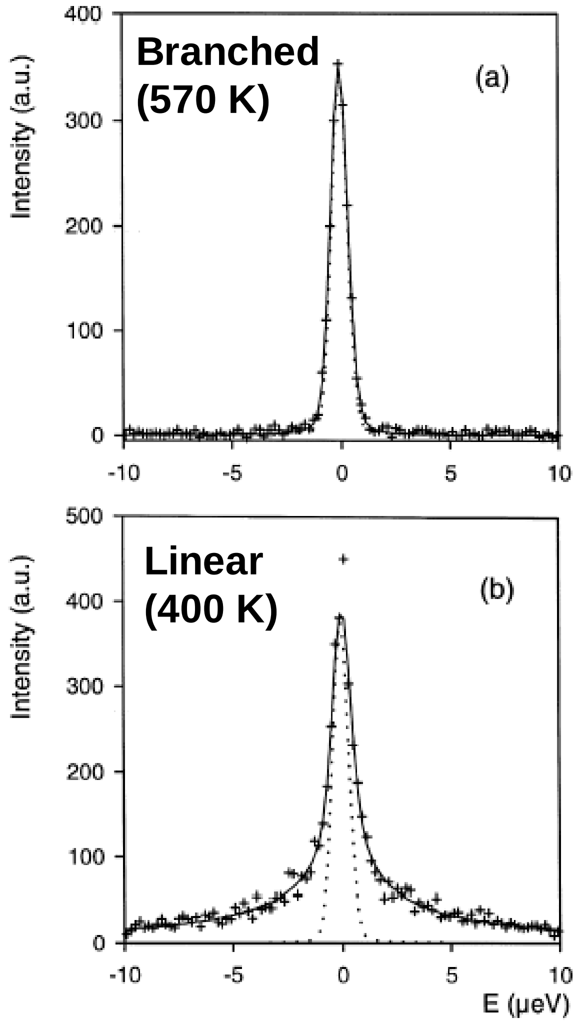
T Mason, SNS

Diffusion in Zeolites – Quasielastic Neutron Scattering (QNS)



View down the 5.5 Å diameter channels of ZSM-5





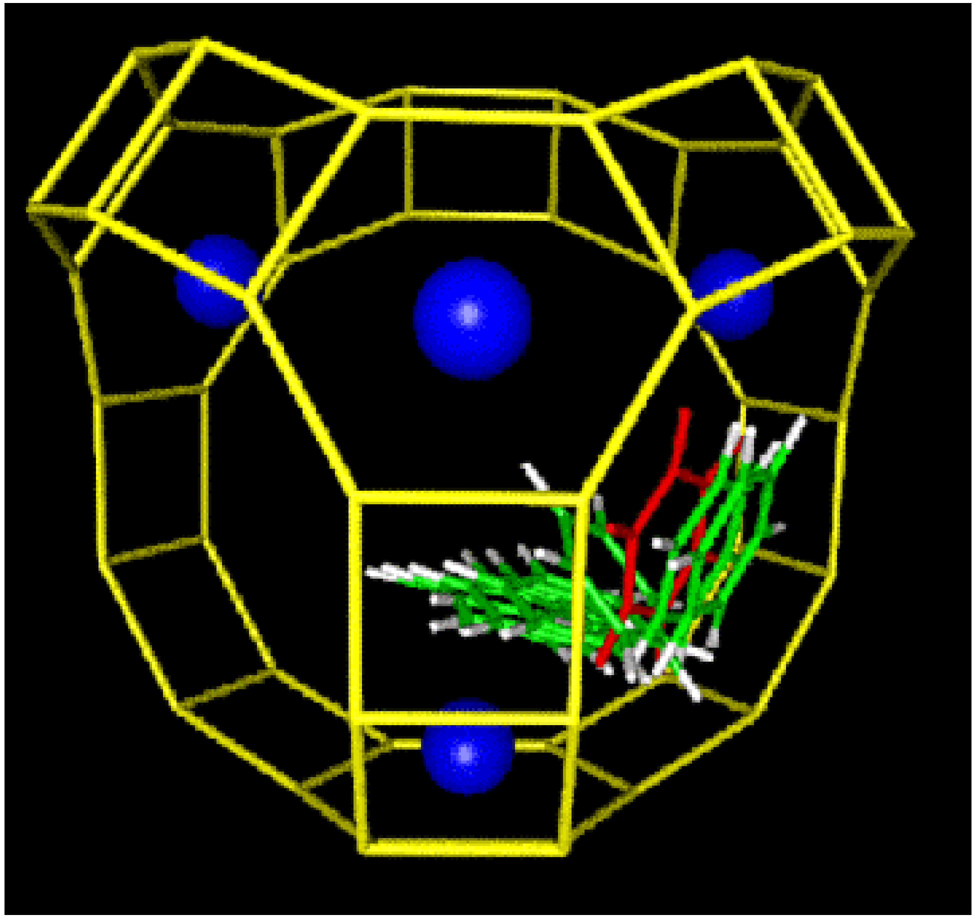
Alkane diffusion in zeolites studied by QNS using the backscattering spectrometer IN-16 at the ILL – H. Jobic, J. of Molecular Catalysis A-**158** (2000) 135-142.

Long n-alkanes diffuse slower then shorter ones with no plateau effect as predicted by simulation methods.

On the microscopic length scale of these measurements, branched alkanes ($CH(CH_3)_3$ – 570 K) diffuse much more slowly then n-alkanes ($CH_3(CH_2)_6CH_3$ – 400 K)

T Mason, SNS

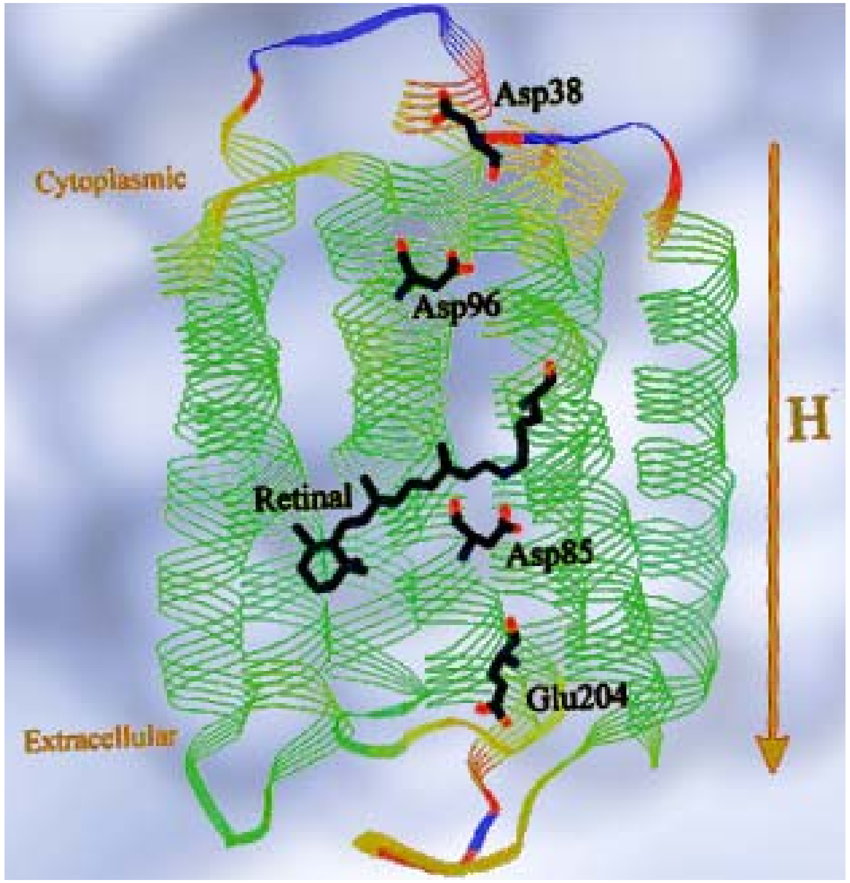
Neutrons measure the Velocity of Atoms



Benzene motion in a zeolite based catalyst

Neutrons follow catalysts in action.

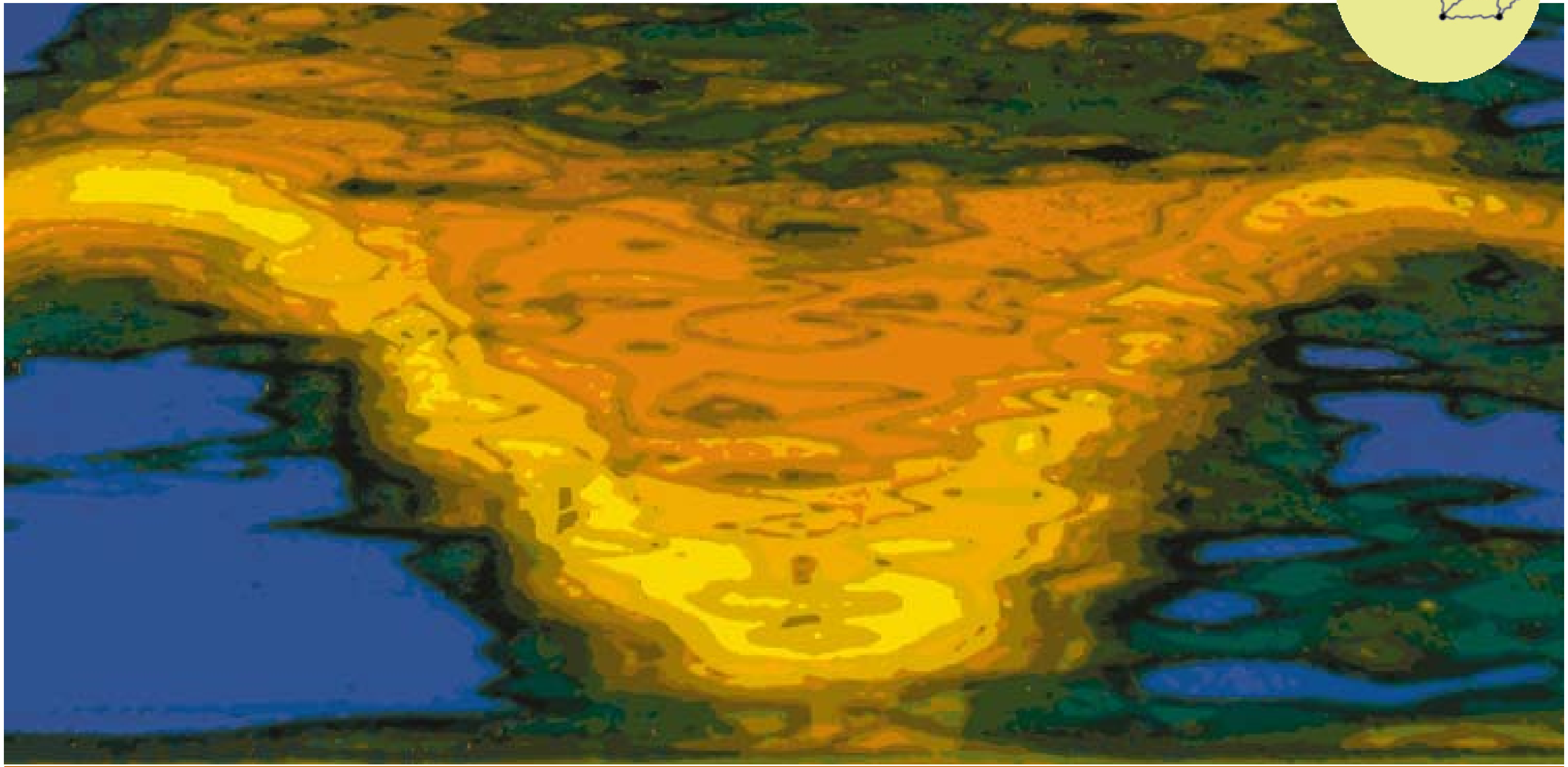
Neutrons measure the Velocity of Atoms



Mechanism of proton pumping

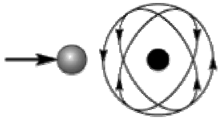
Transport through a biological membrane.

Neutrons measure Motion of Elementary Magnets



The motions of elementary magnets tell us on the origins of magnetic properties.

Uniqueness of Neutrons



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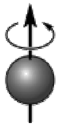

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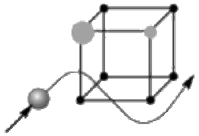

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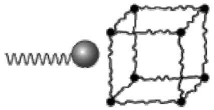

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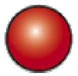
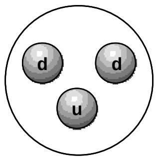


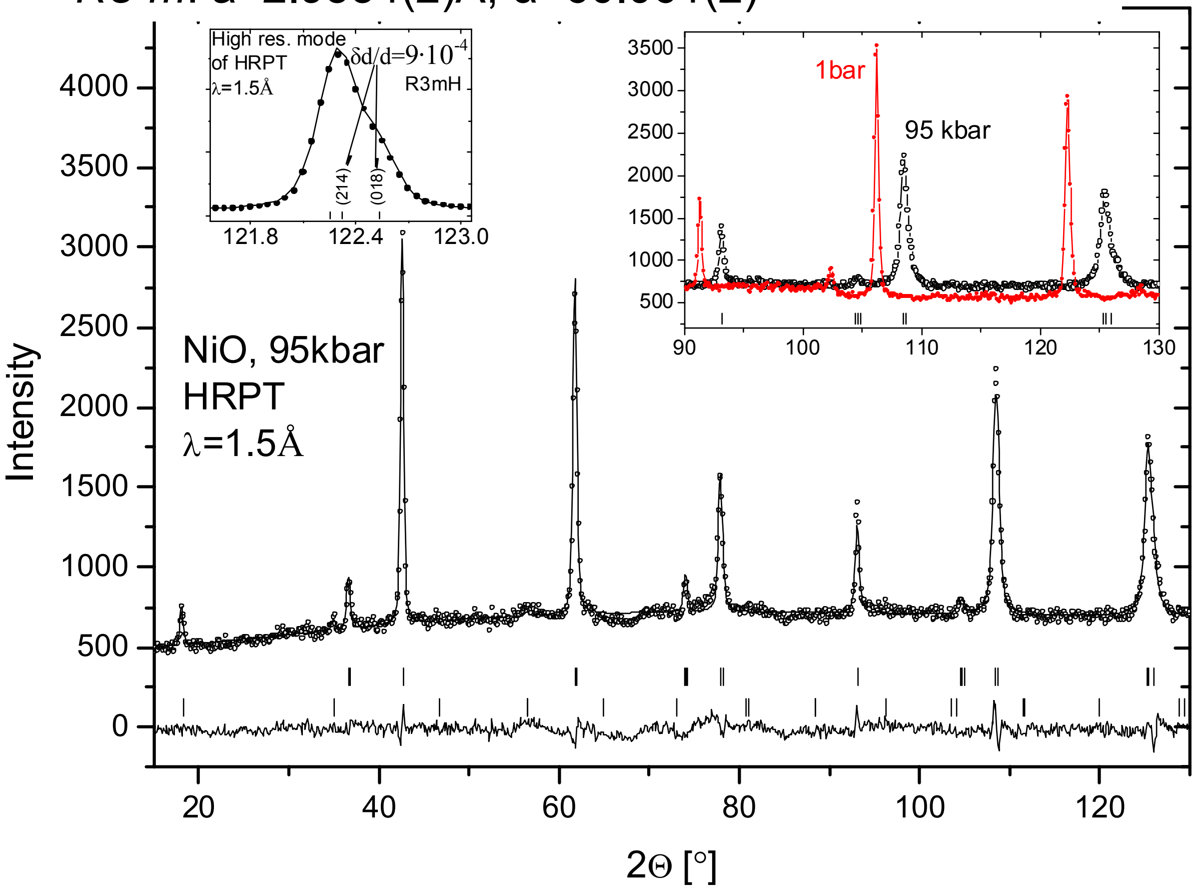
5. **Neutrons penetrate deep into Matter**



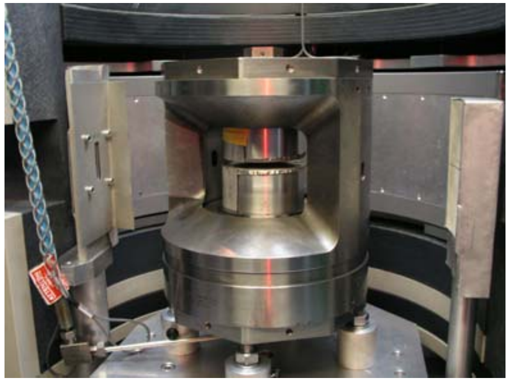
6. Neutrons are Elementary Particles

Lattice distortion and magnetic structure in NiO under high pressures (up to 130kbar)

@ p=1bar: μ_{Ni}=1.73(9) μ_B, k =[½ ½ ½] in *Fm3m*
R3-m: a=2.9534(2)Å, α=60.061(2)°

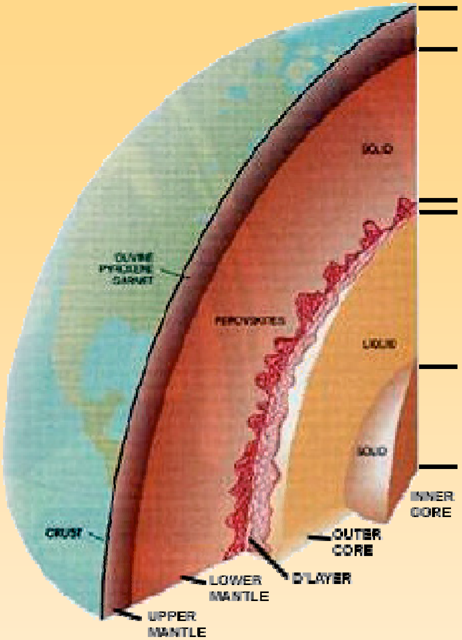


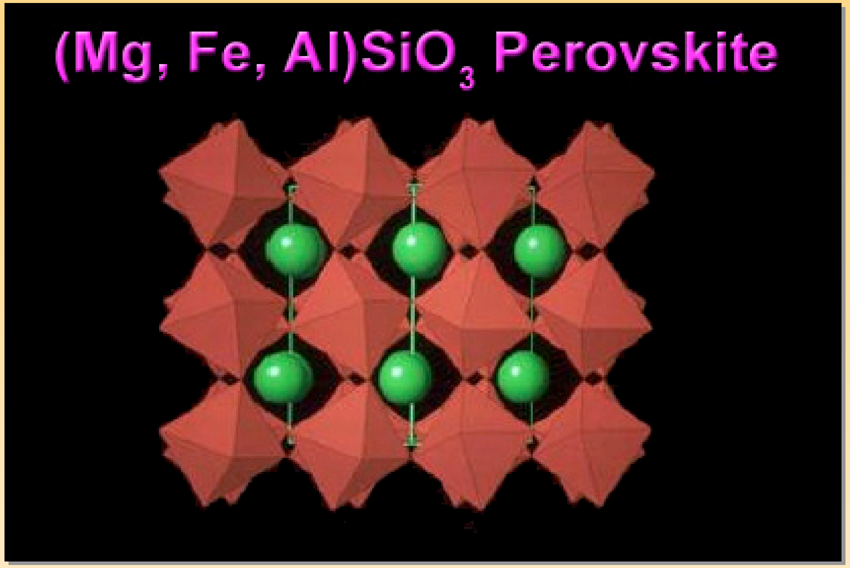
S. Klotz, Th. Strässle, G. Rousse, G. Hamel, V. Pomjakushin, *APL 2005.*



V. Pomjakushin PSI

Structure at Extremes of Pressure and Temperature





Most abundant mineral in the planet

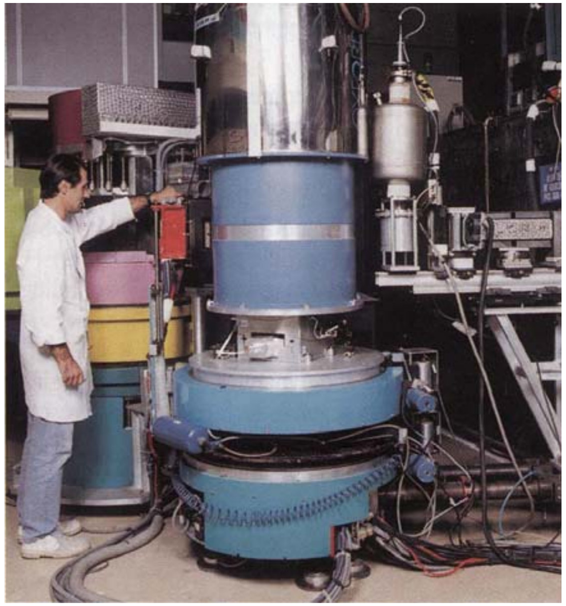
Pressure cell of the type to be employed on SNAP (Spallation Neutrons and Pressure) beamline

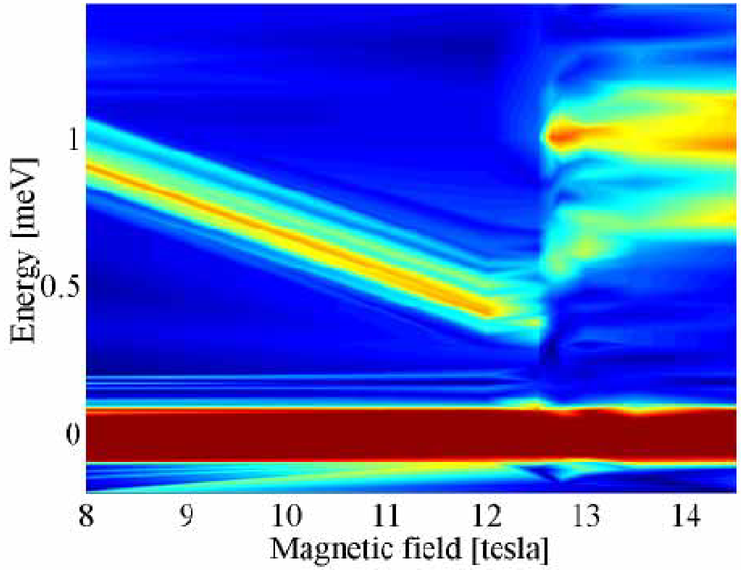
T Mason, SNS

Sample environment – Magnetic fields

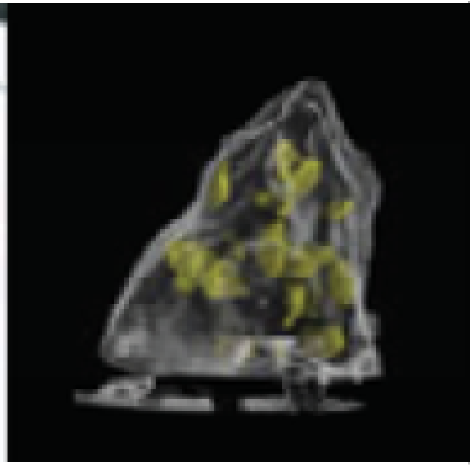
The neutron is highly penetrating -

enabling studies of samples in containers and complex sample environment…



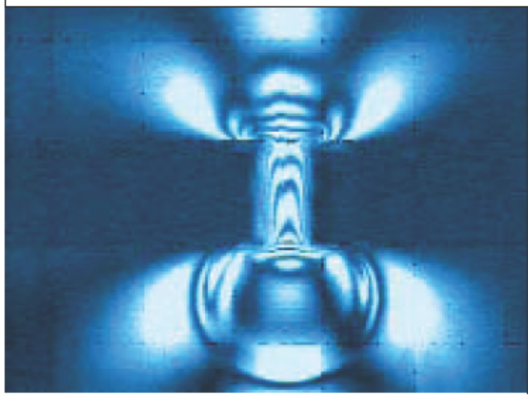


Neutrons penetrate deep into Matter



Neutrons can see a red rose inside a lead flask or fossilized Arauc leaves inside an Antarctic rock

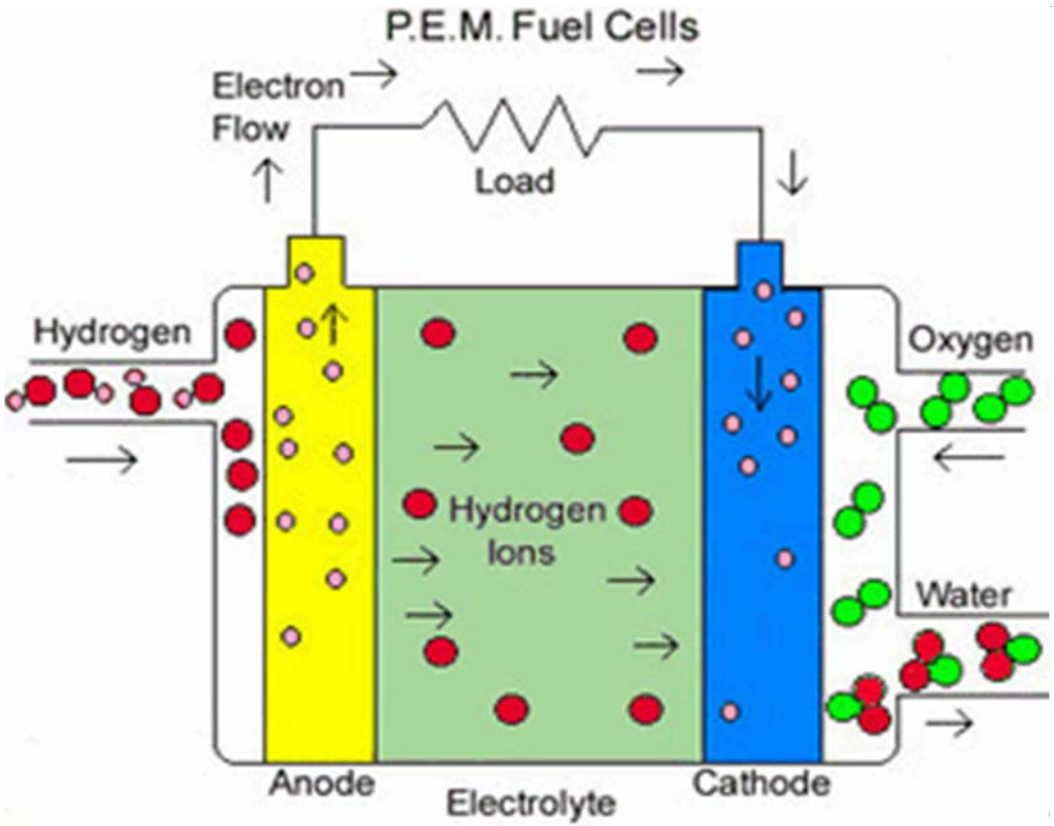
Materials and processing

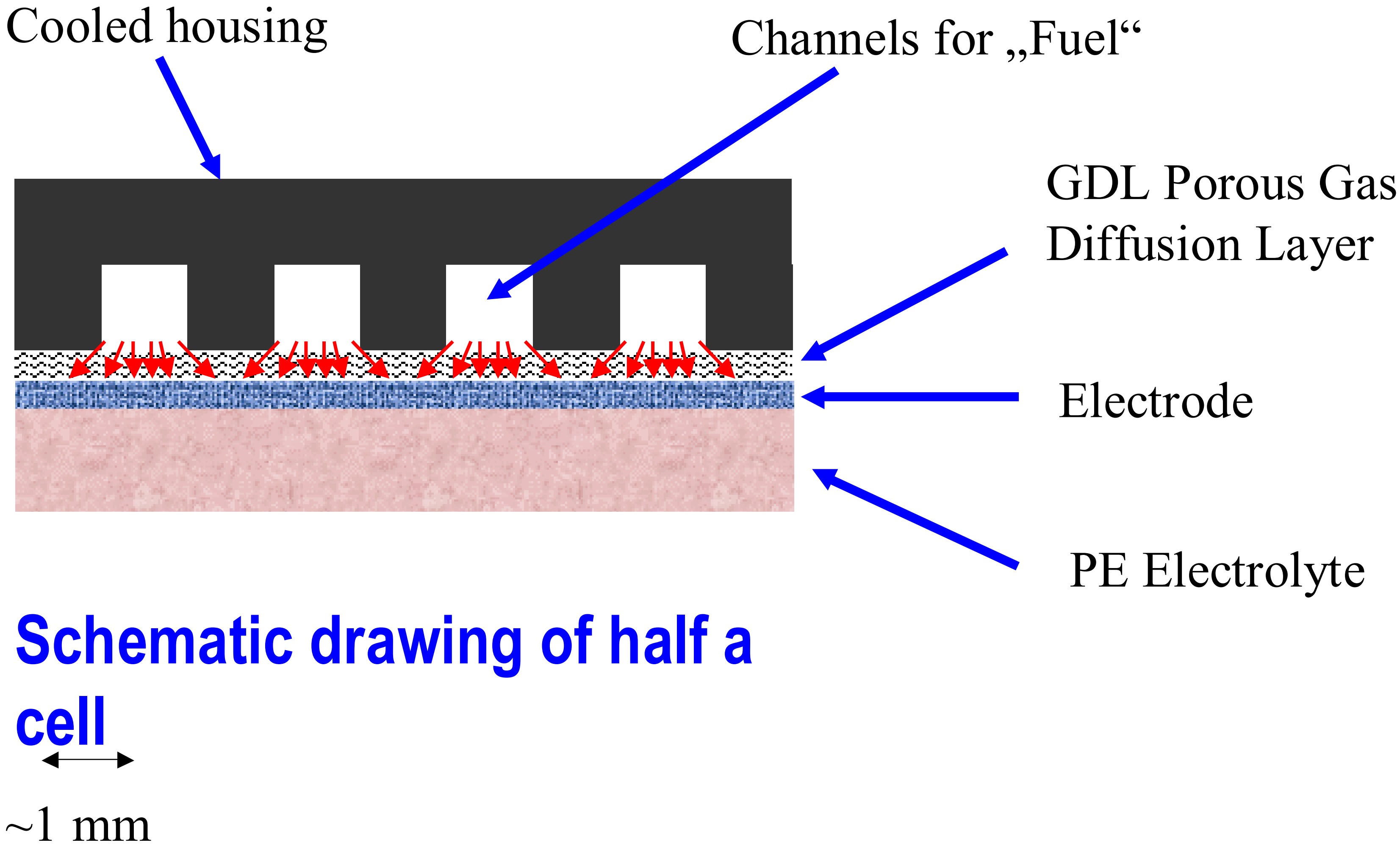


- Processing of soft solids and complex fluids in extruders, mixers, pipe flow and micro-fluidics
- Controllable rheology for lubricants and oil extraction
- Structural integrity and safety: remediation of residual stresses in alloys, composites and welds
- Light weight, high strength, alloys and composites; superconducting wires, bulk amorphous alloys
- In-situ measurements to understand materials synthesis, processing and treatments

Proton Exchange Membrane fuel cell

~ 80 C, polymer electrolyte - thin permeable sheet.

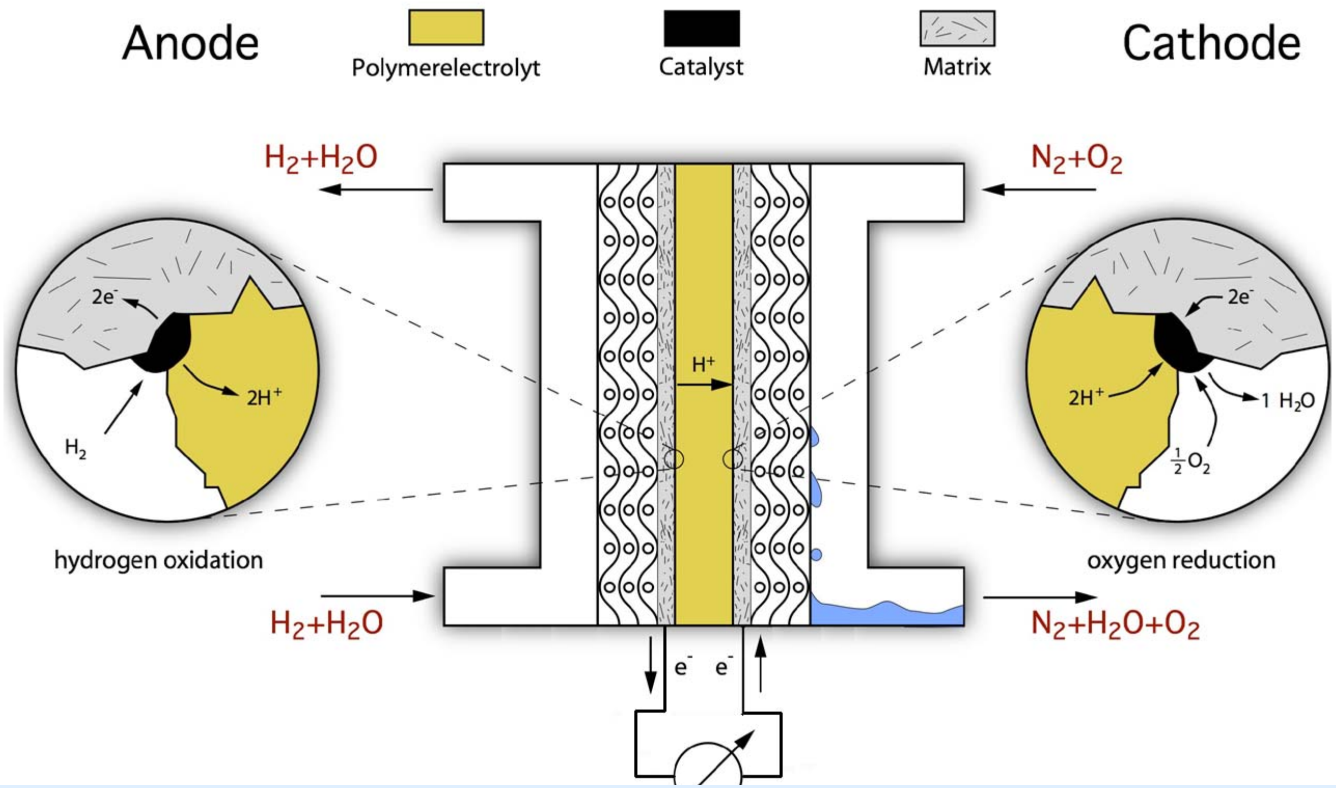




Schematic drawing of half a cell

PEFC

D Kramer, PSI



The reaction product is water

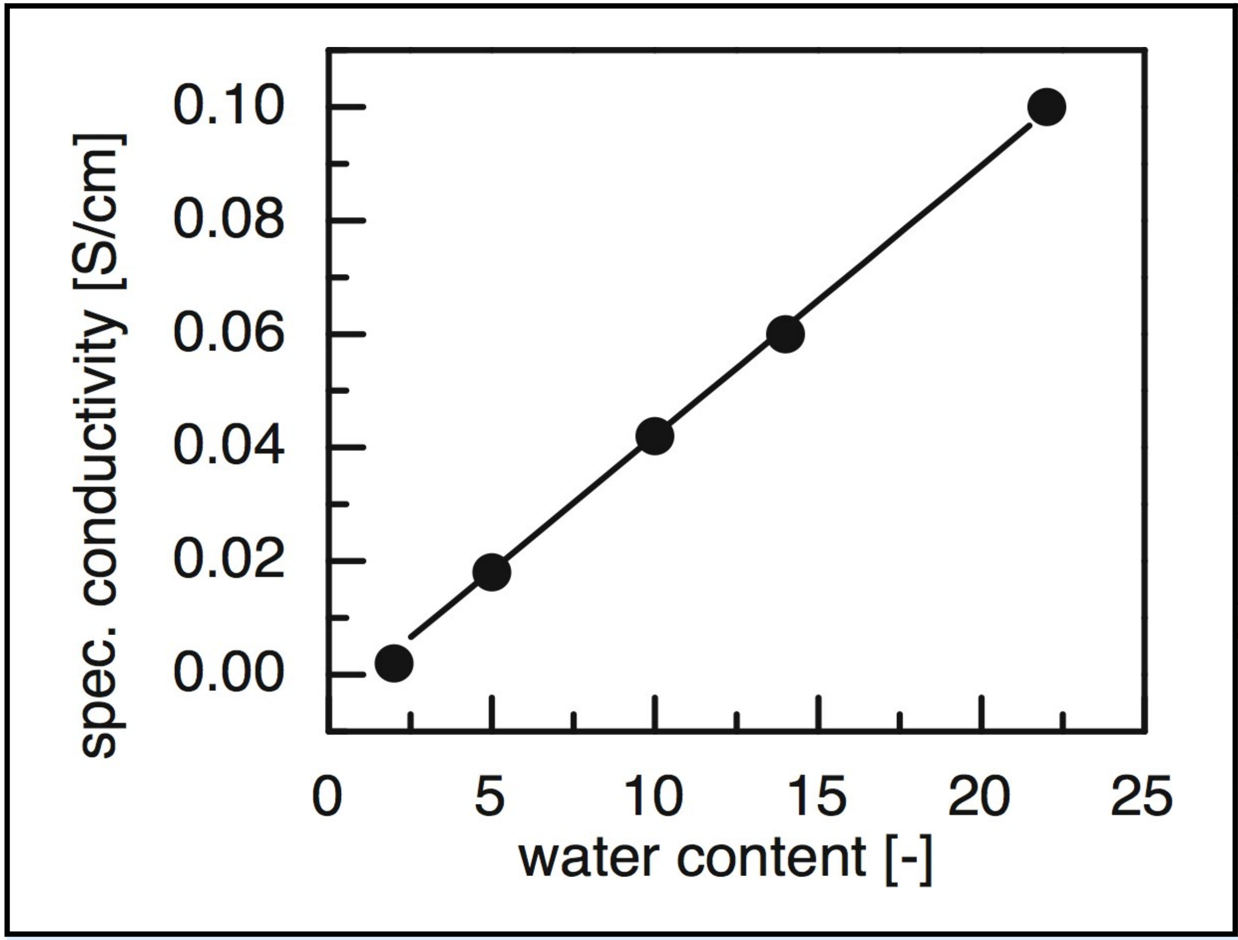
Today's electrolyts require water for high conductance

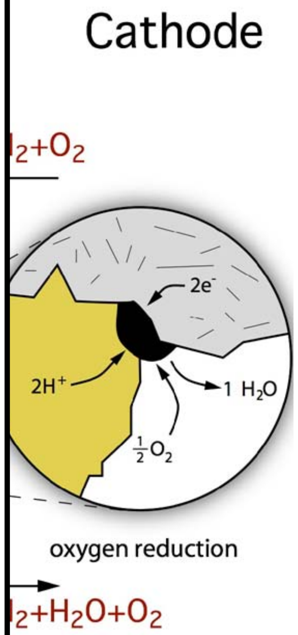
Under low stochiometries the saturation pressure is easily reached and liquid blocks the gas supply

PAUL SCHERRER INSTITUT

PEFC

D Kramer, PSI

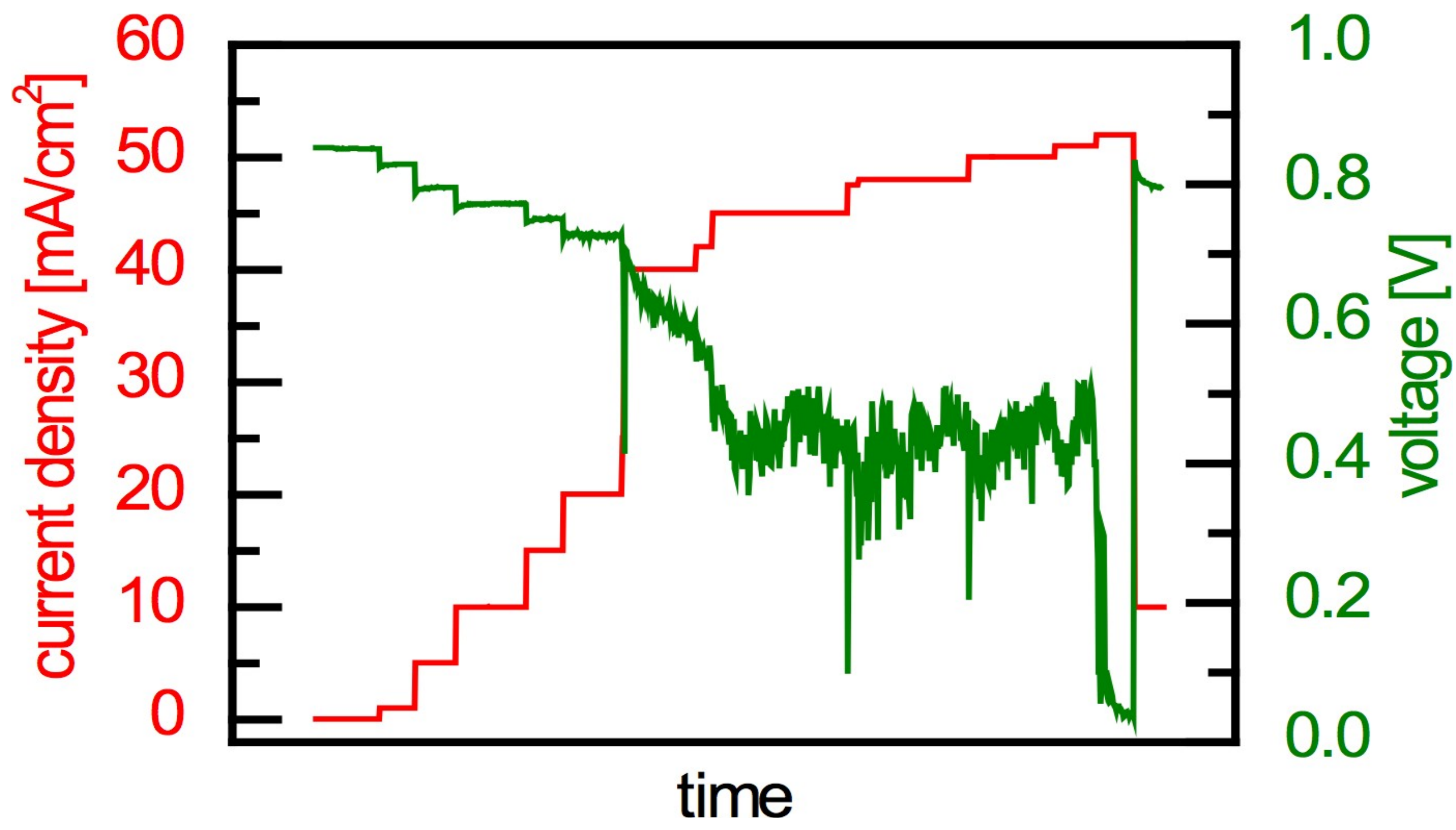




Under low stochiometries the saturation pressure is easily reached and liquid blocks the gas supply

PEFC

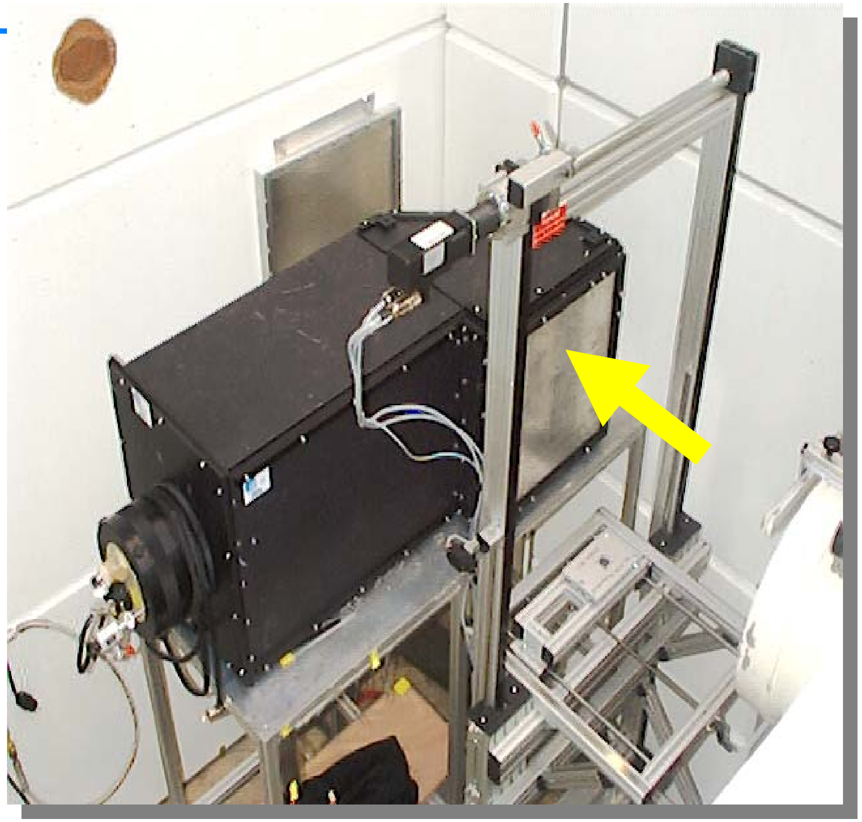
D Kramer, PSI

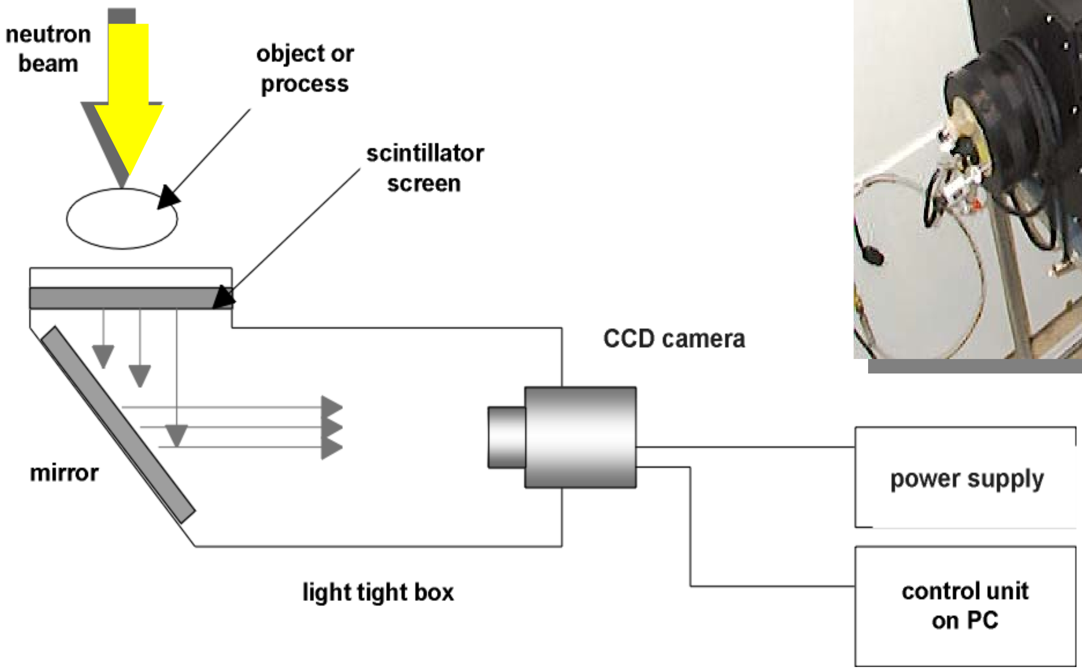


E Lehmann, PSI

CCD-camera detector

neutrons are hitting the scintillator and the emitted light will be detected by the high sensitive camera.





Li^6 doped ZnS (better yield and less gamma sensitive)

or Gd oxy sulfide (for simultanous neutrons and gamma/x-ray measurements.

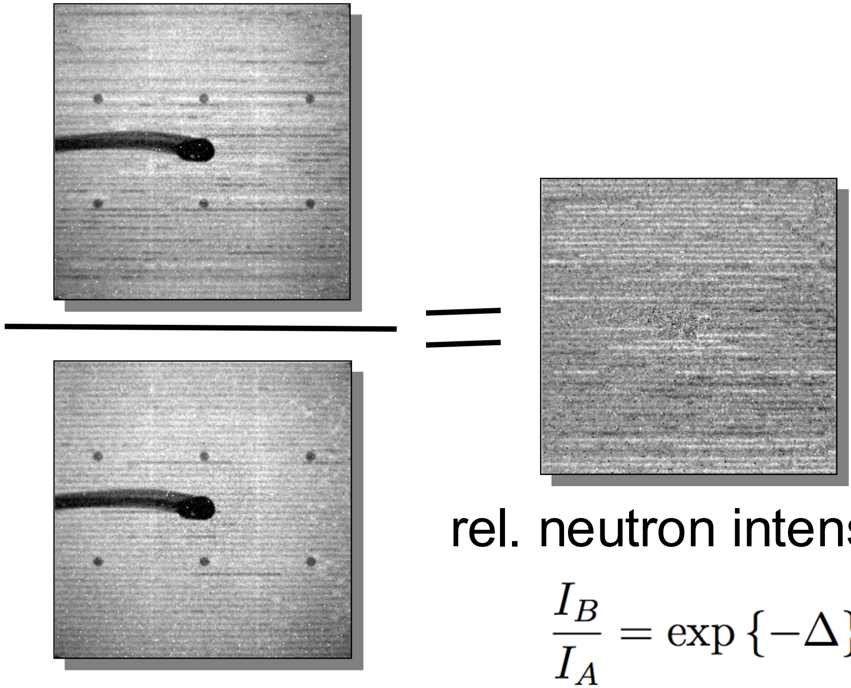
D Kramer, PSI

FC under load

$$I_B = I_0 \cdot \exp\left\{-\left(\sum a_{cell} + \Delta\right)\right\}$$

FC at OCV

$$I_A = I_0 \cdot \exp\left\{-\sum a_{cell}\right\}$$



rel. neutron intensity

$$\frac{I_B}{I_A} = \exp\{-\Delta\}$$

Present practical sensitivity
10 μm of water

D Kramer, PSI

FC under load

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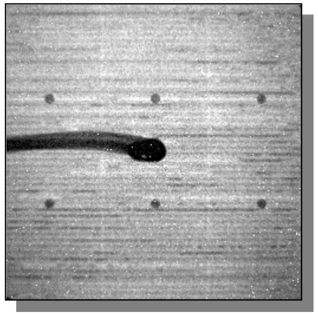

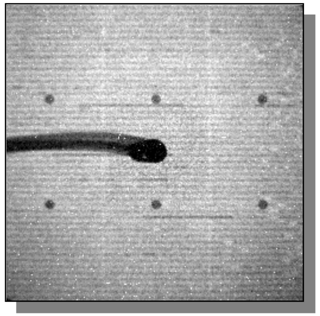

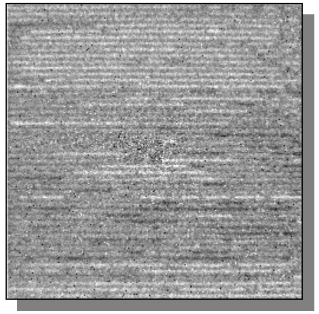

FC at OCV

$$I_A = I_0 \cdot \exp\left\{-\sum a_{cell}\right\}$$

OCV = Open Cell Voltage – the cell is at temperature but dry – reference measurement

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D Kramer, PSI

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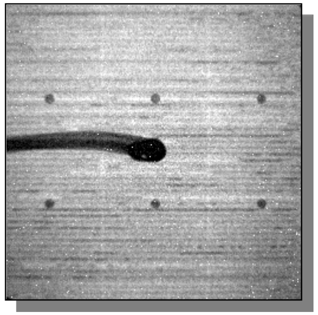

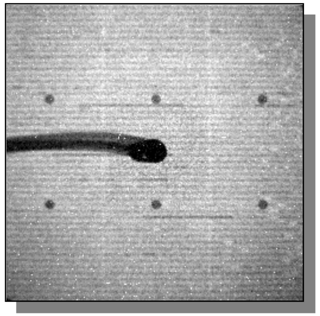

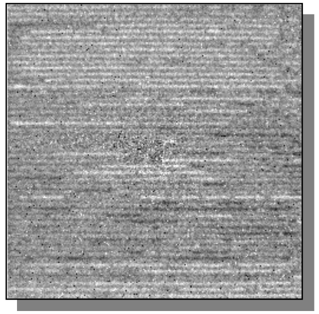

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Present practical sensitivity
10 μm of water

Gas flow rate up to 10 m/s
i.e down to ≈ 10 ms from side to side i.e. temporal average

D Kramer, PSI

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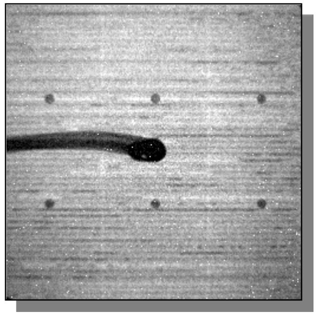

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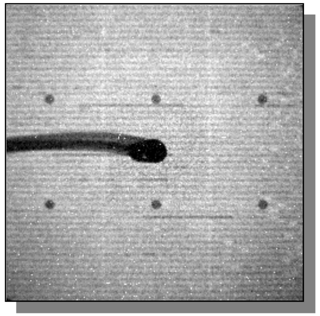
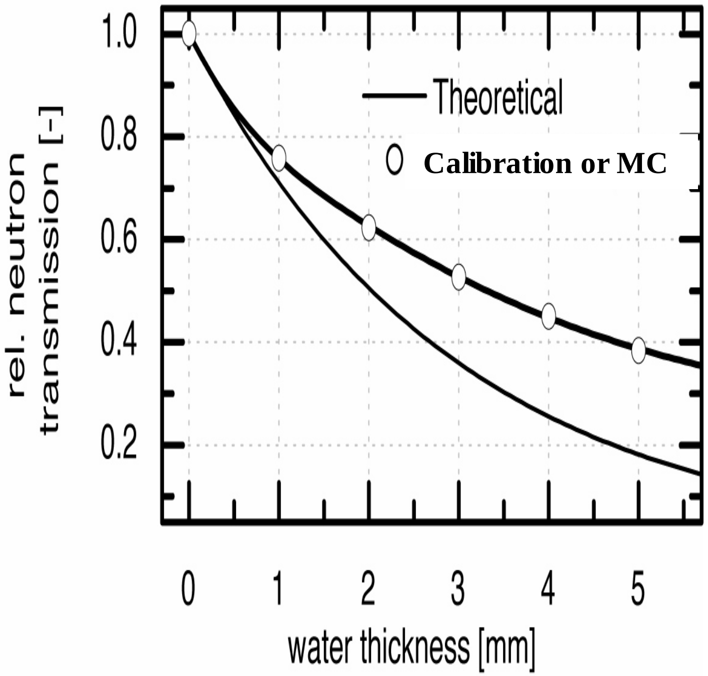


OCV = Open Cell Voltage – the cell is at temperature but dry – reference measurement

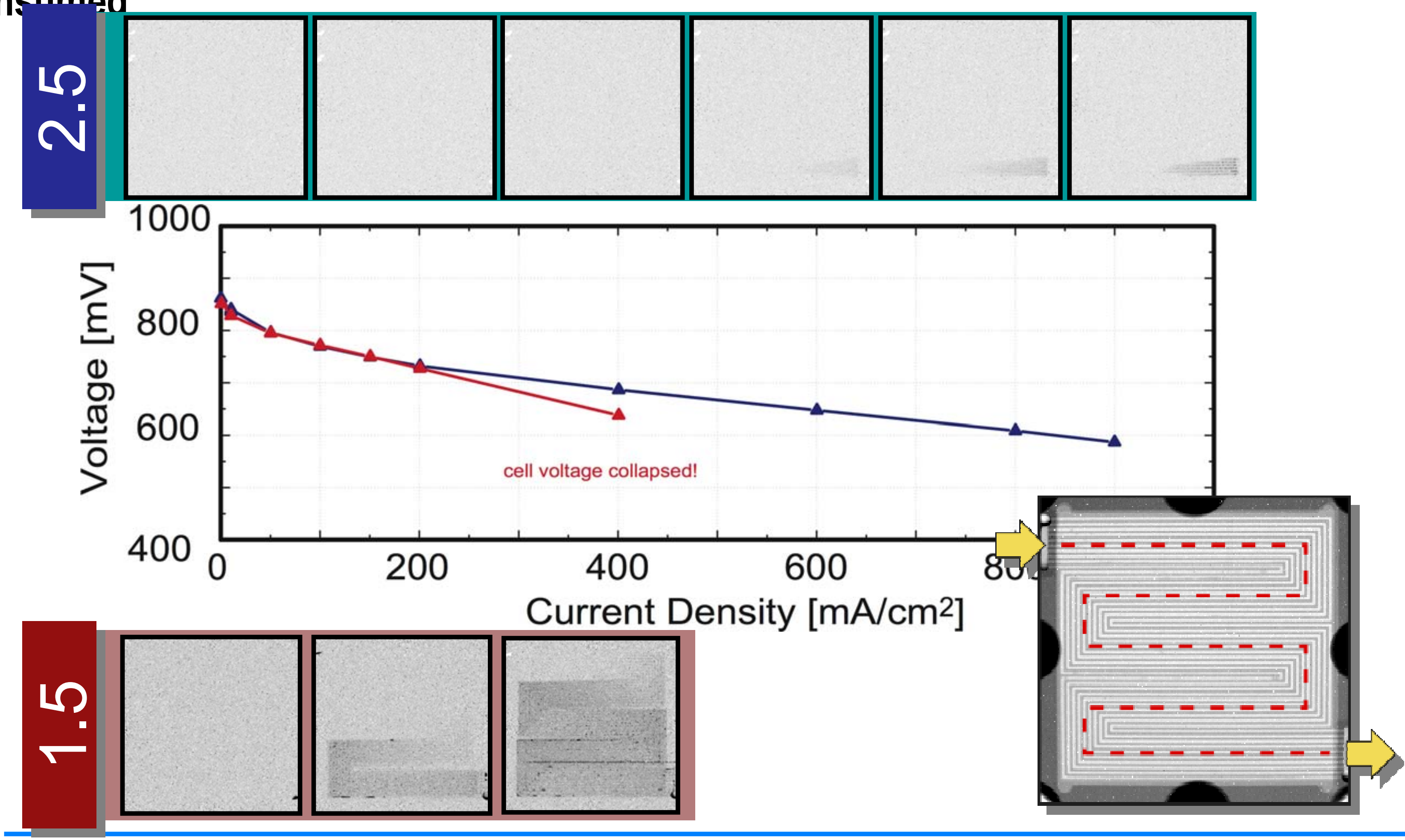


Gas flow rate up to 10 m/s
i.e down to ≈ 10 ms from side to side i.e. temporal average

Present practical sensitivity
10 μm of water

D Kramer, PSI

PEFC flooding – Total amount of Oxygen in the inlet gas / Amount of Oxygen consumed



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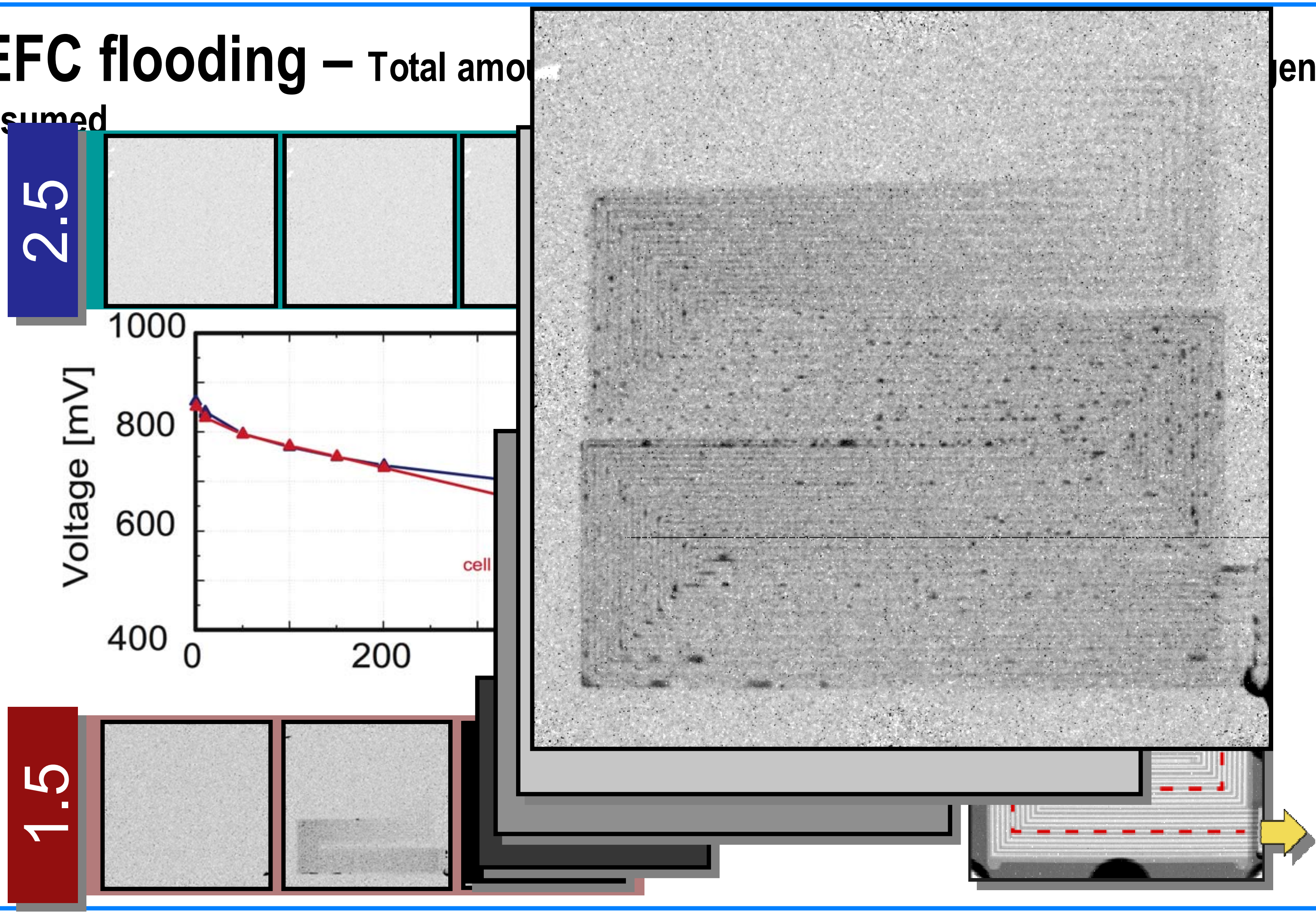
PSI

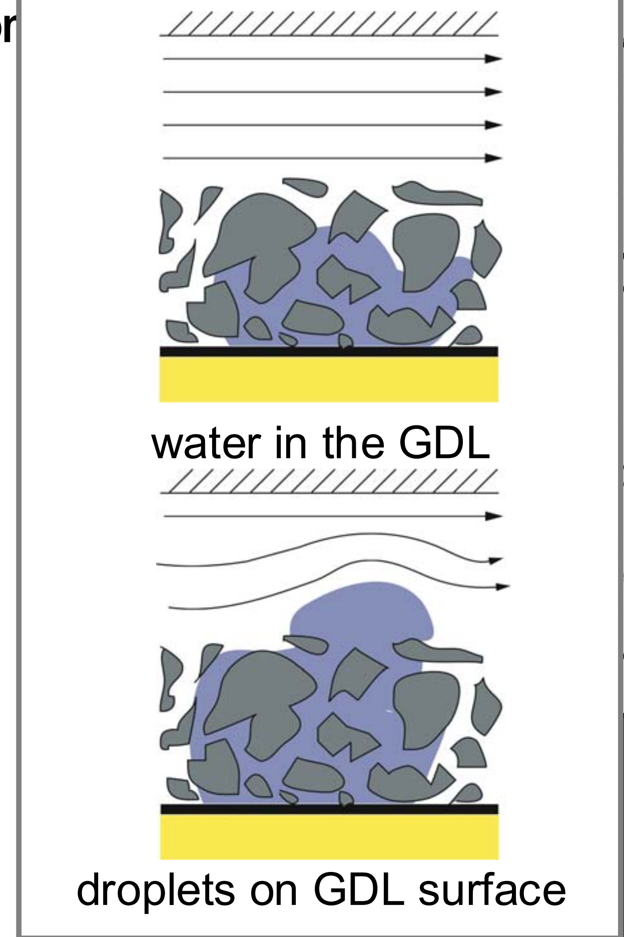
D Kramer, PSI

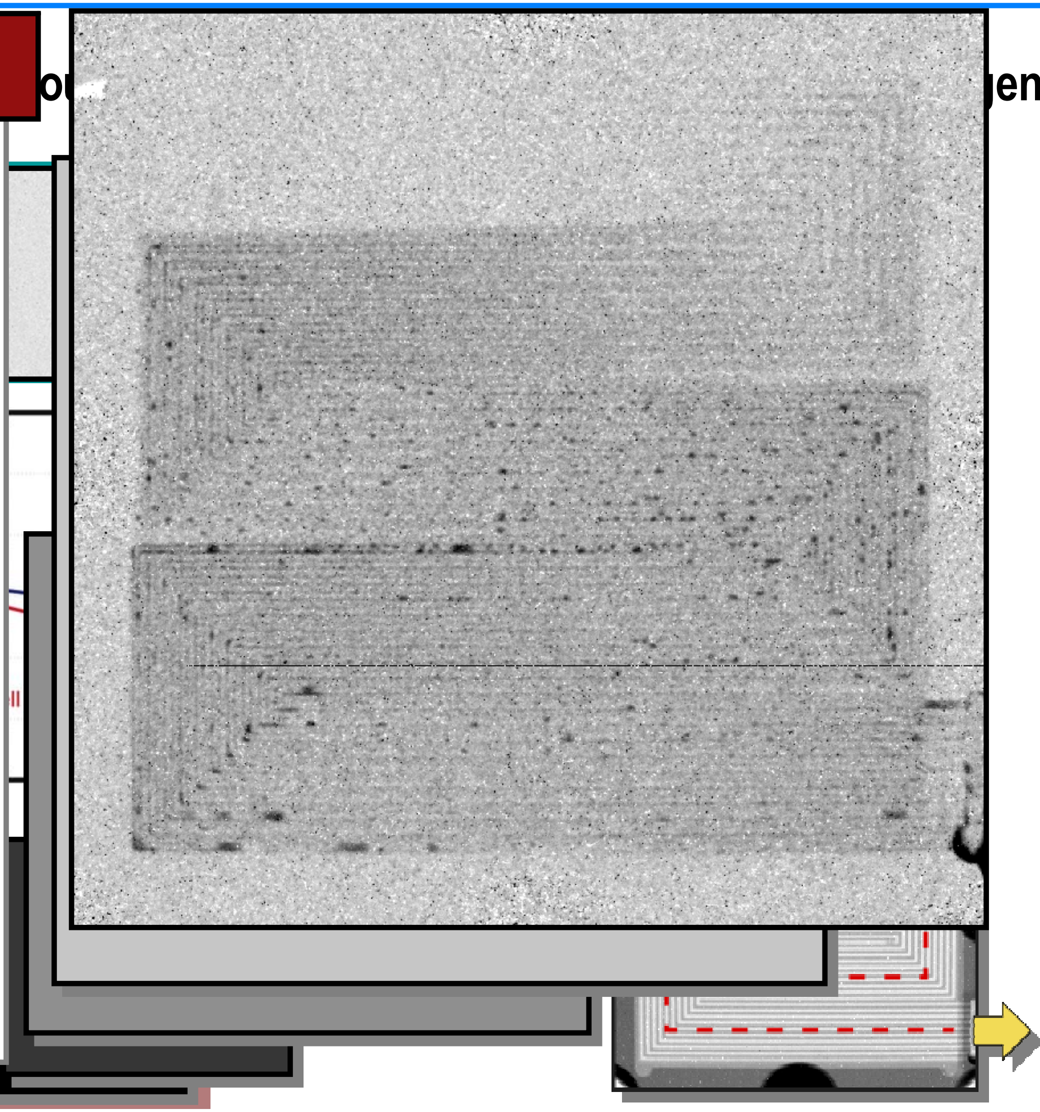
PEFC flooding – Total amo... ...gen consumed



D Kramer, PSI

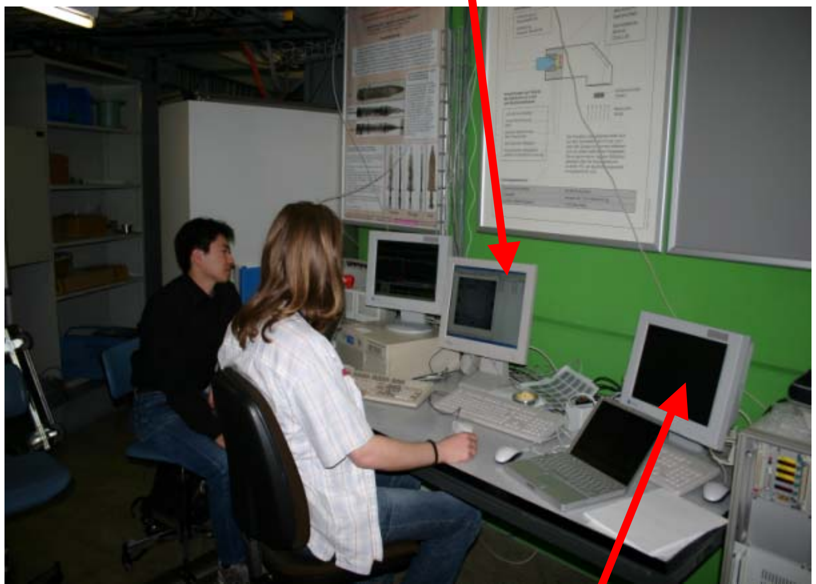
Kinds of liquid

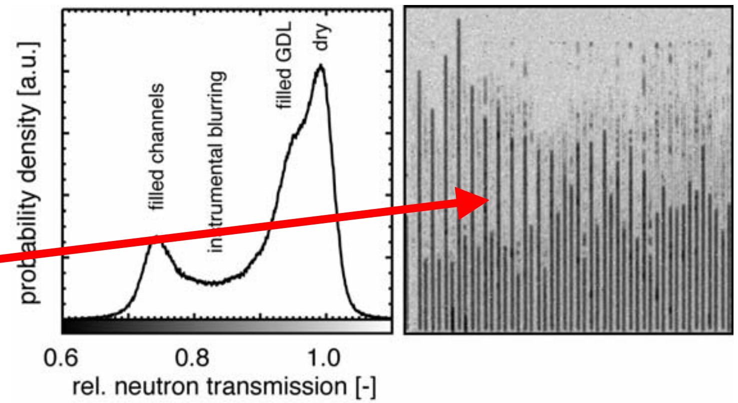




D Kramer, PSI
Nissan

Experiment





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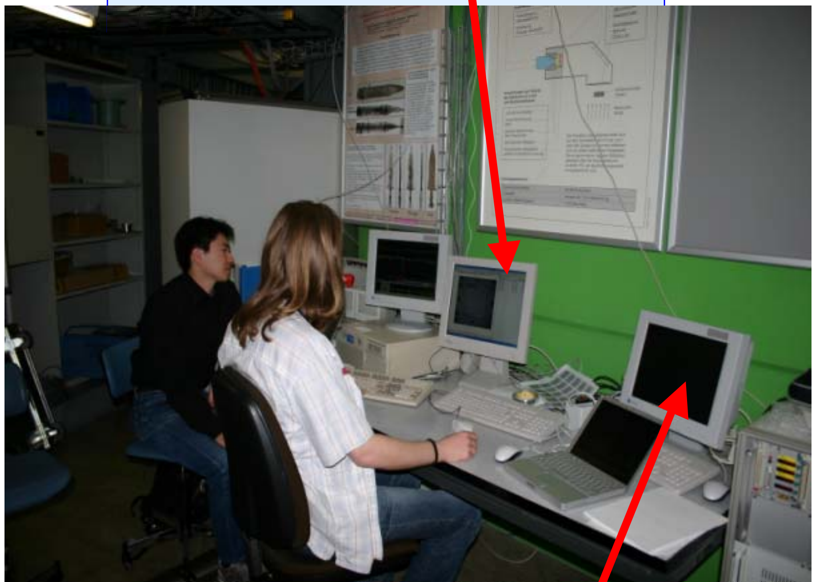
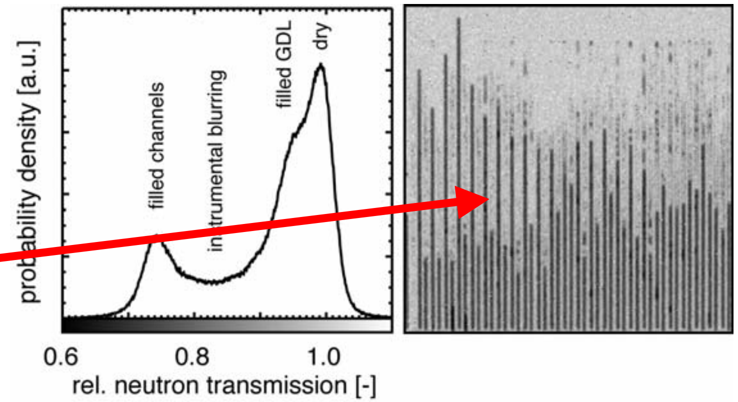
D Kramer, PSI
Nissan

Experiment

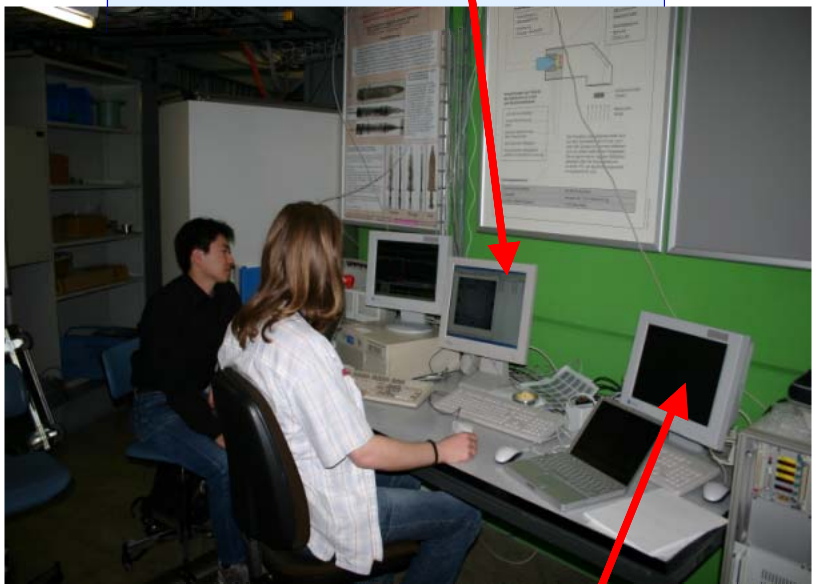


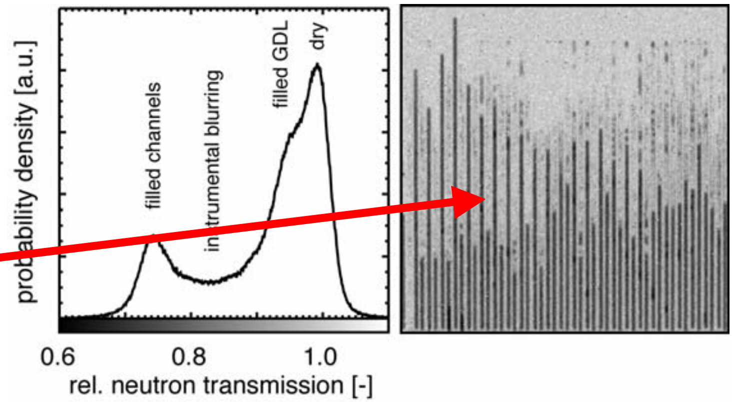


D Kramer, PSI
Nissan

Experiment

Fuel cell Control parameters:





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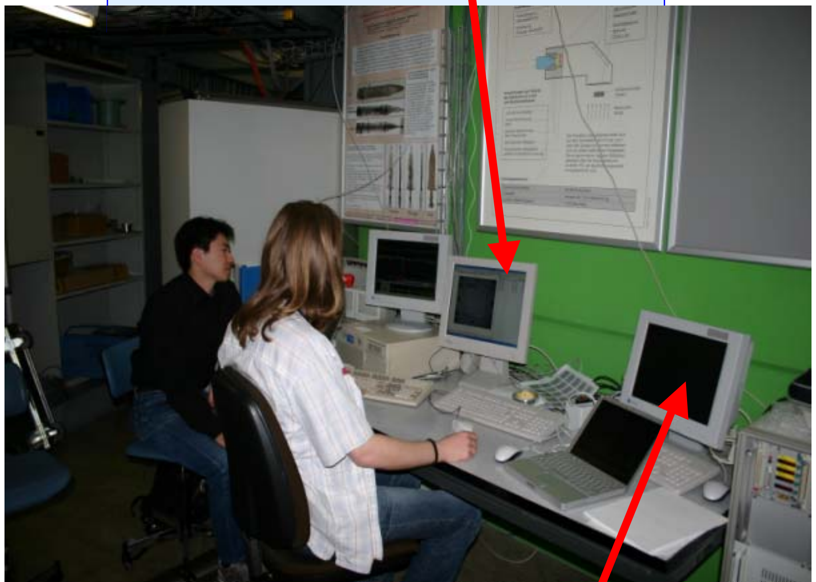
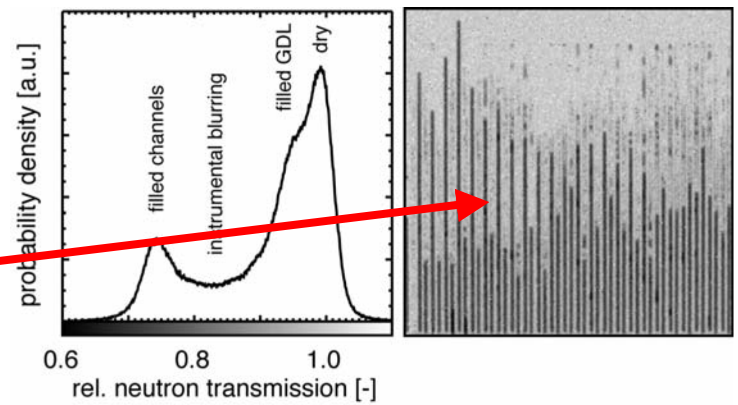
Nissan

Experiment

Fuel cell Control parameters:

- Gas flow rate



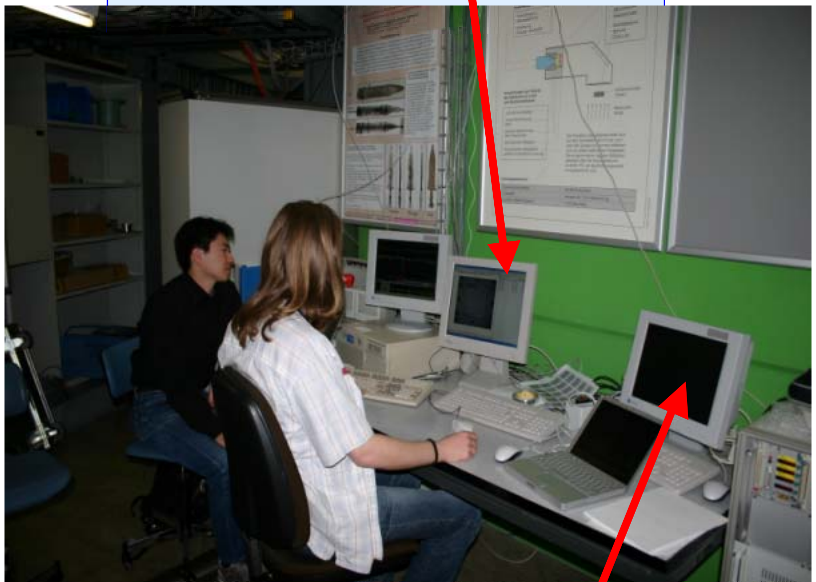


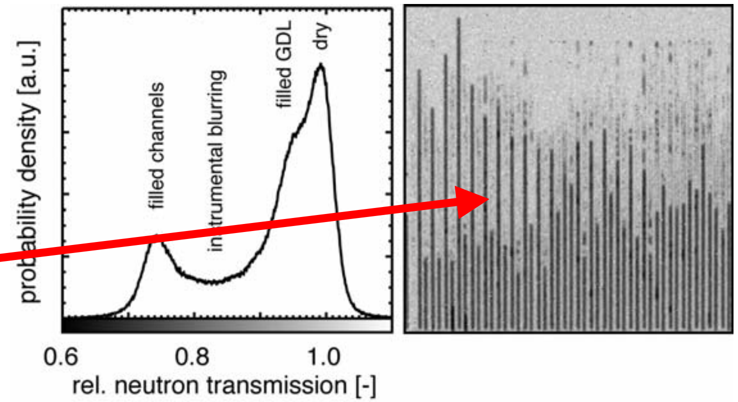
D Kramer, PSI
Nissan

Experiment

Fuel cell Control parameters:

- Gas flow rate
- Temperature





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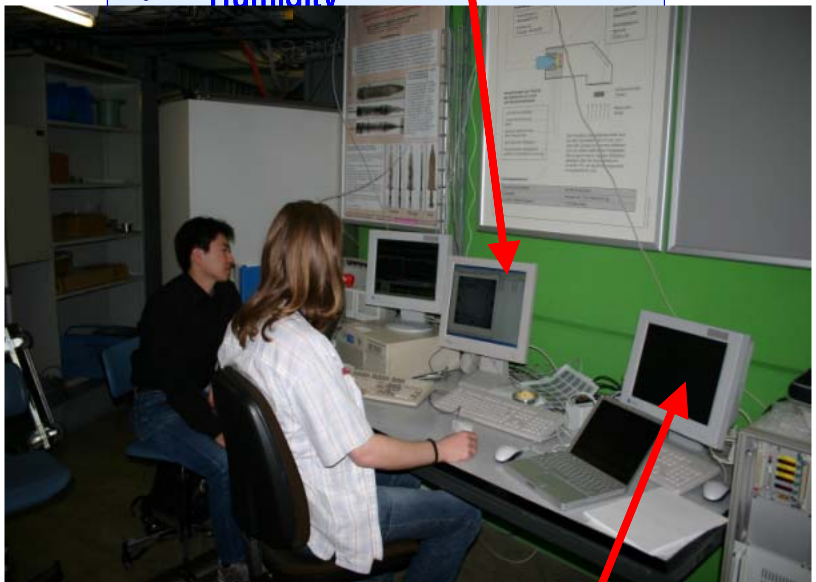
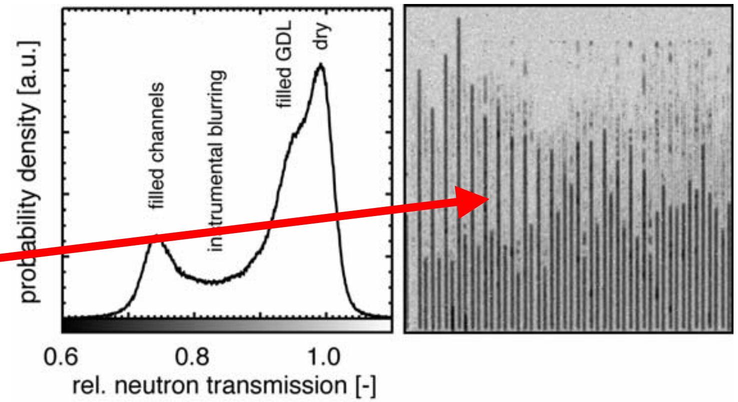
D Kramer, PSI
Nissan

Experiment

Fuel cell Control parameters:

- Gas flow rate
- Temperature
- Humidity





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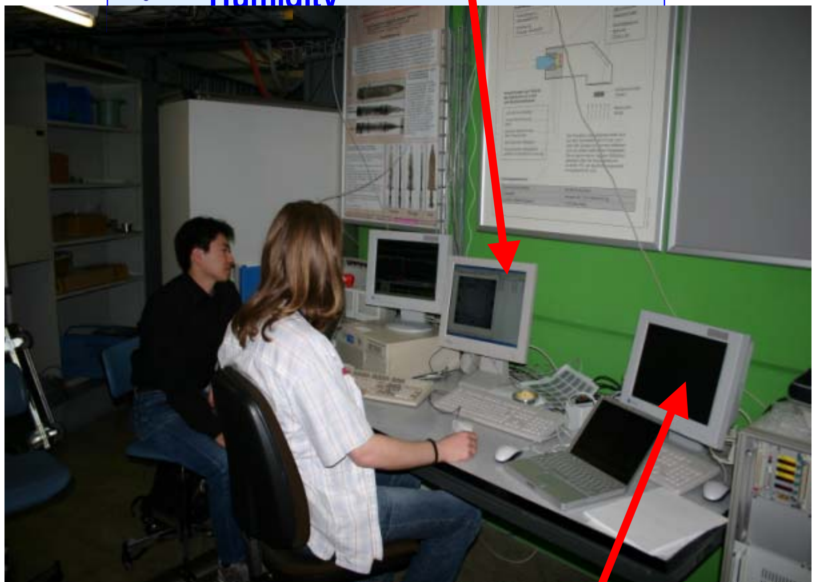

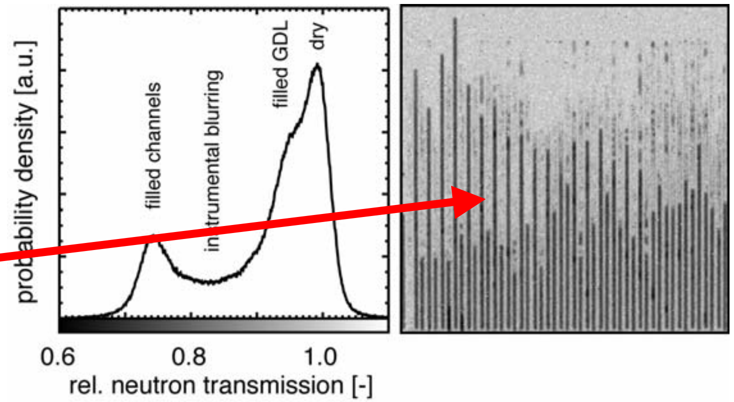

PAUL SCHERRER INSTITUT

D Kramer, PSI
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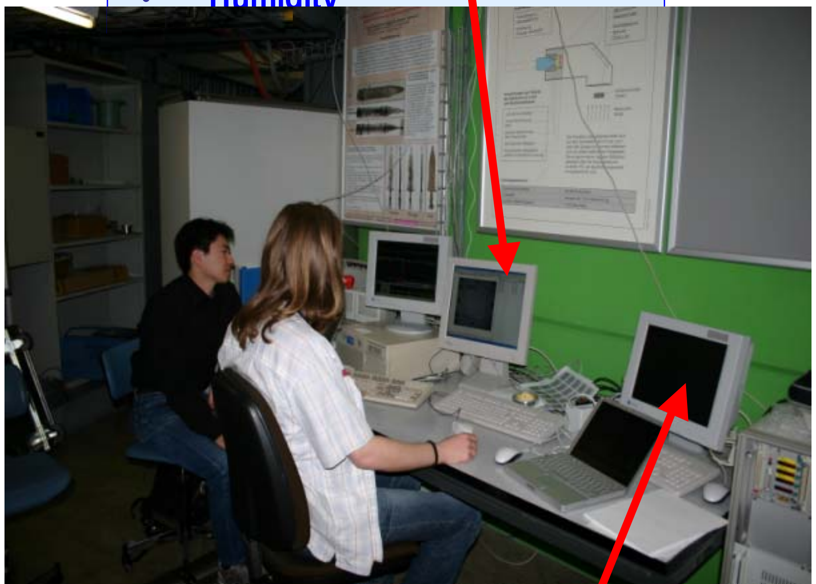
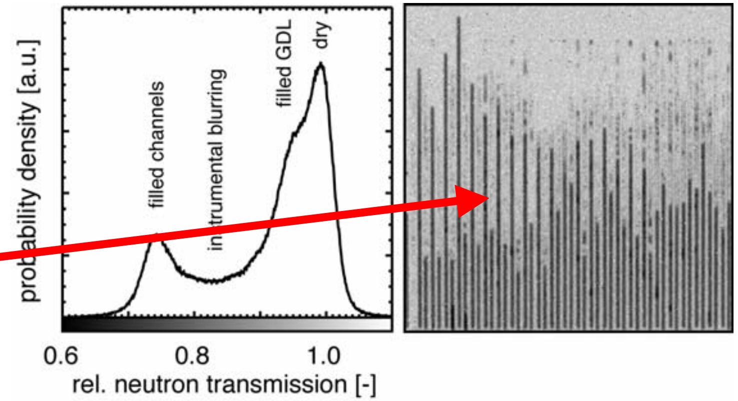


Neutron radiography:

•Exposure time or frames/s

•Online analysis



PAUL SCHERRER INSTITUT

Today Future perspectives

Spatial resolution:

today ≈ 250-400 μm

Sensitivity:

today ≈ 10 μm water layer

Temporal resolution:

7.5 frames/s

If we want 1 frame to integrate over max 1 mm then this corresponds to

0.0075 m/s

E Lehmann, PSI

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PAUL SCHERRER INSTITUT PSI

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→ 50 µm → 10 µm →

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PAUL SCHERRER INSTITUT

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Wanted sensitivity

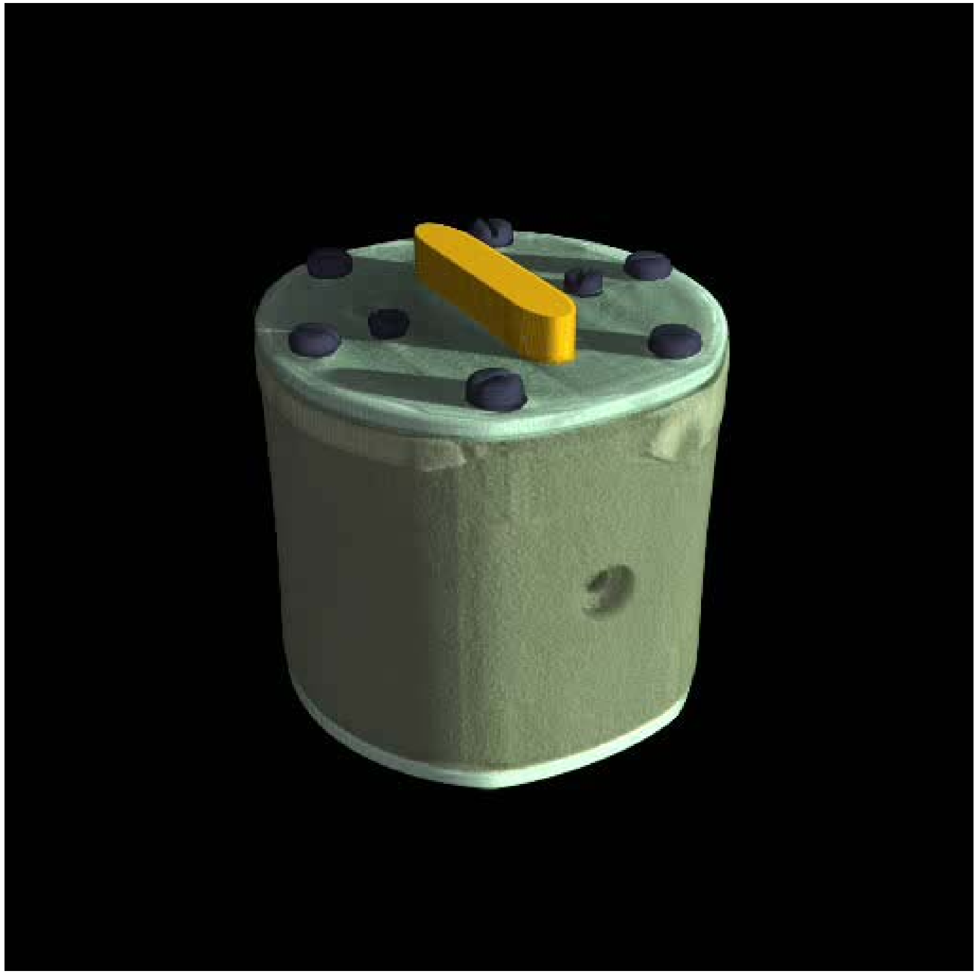
→1 μm water layer

Gas flow rate in cell → 10 m/s

Droplet flow rate expected to be much smaller – but how much?

E Lehmann, PSI

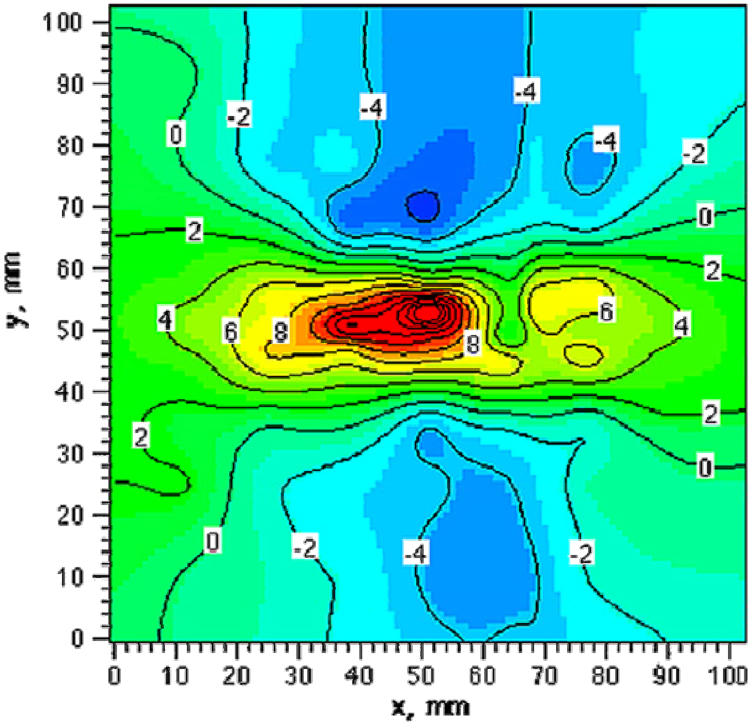
Tomography



A burned fuse!

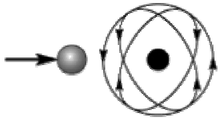
E Lehmann, PSI

Neutrons penetrate deep into Matter

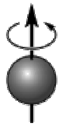


The aircraft of tomorrow: welding instead of rivets.

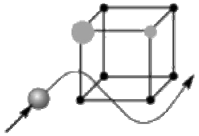
Uniqueness of Neutrons



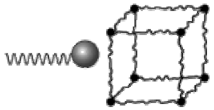
1. **Neutrons see the Nuclei**



2. **Neutrons see Elementary Magnets**

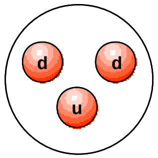


3. **Neutrons see Light Atoms next to Heavy Ones**



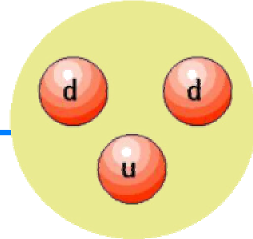
4. **Neutrons measure the Velocity of Atoms**

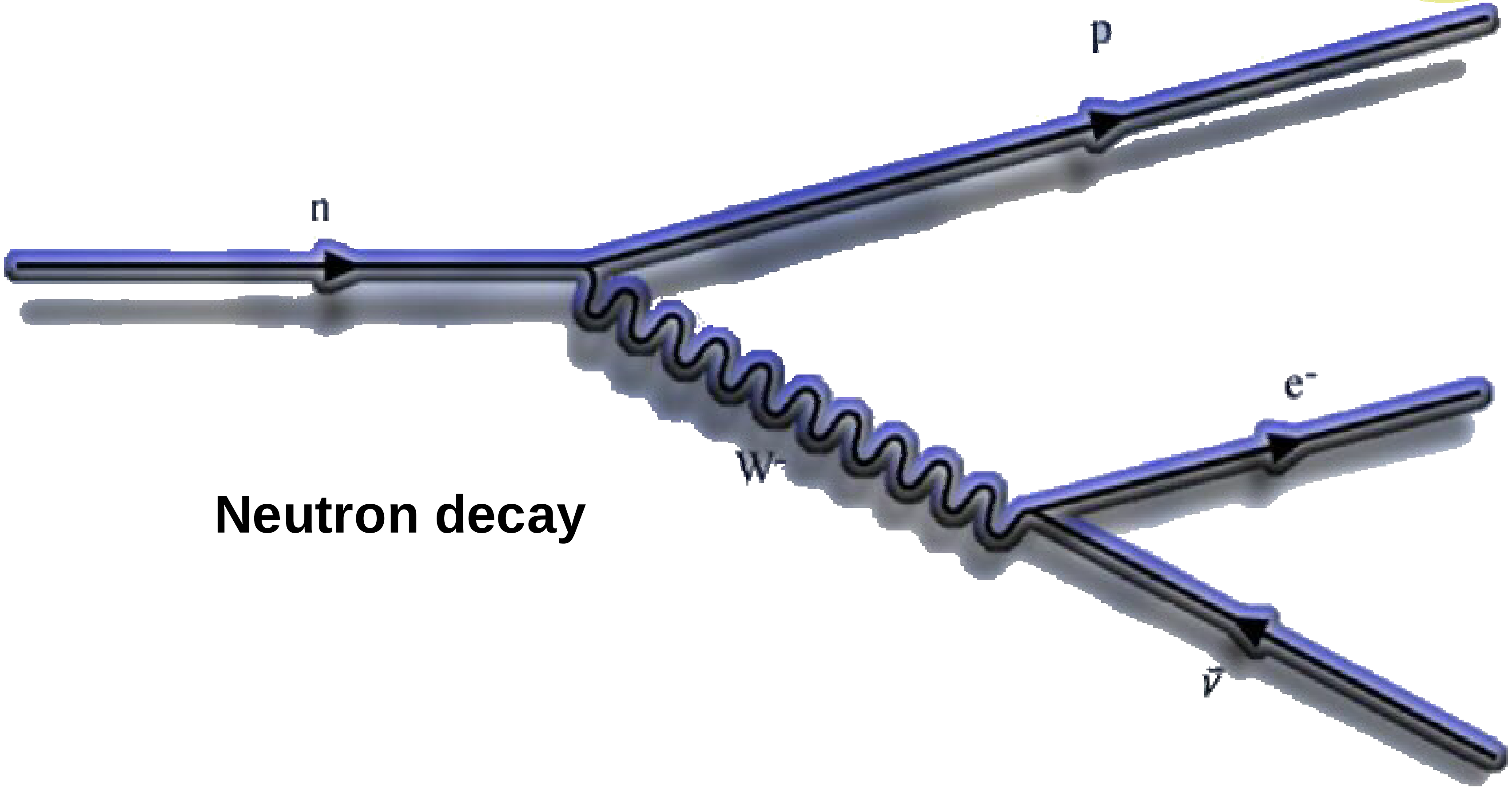
5. **Neutrons penetrate deep into Matter**



6. **Neutrons are Elementary Particles**

Neutrons are Elementary Particles





Neutron decay

Neutron physics elucidates elementary forces of nature.

Useful Neutrons

Neutron and Muon portal – a key web-site

The key web-site for information on and links to neutron and muon sources World-wide is:

http://www.neutron-eu.net/

This site also contains information on how to get access to the European Facilities