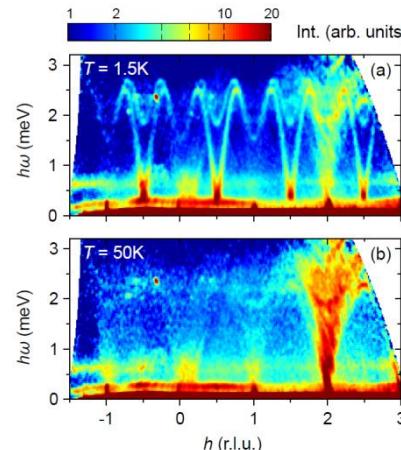
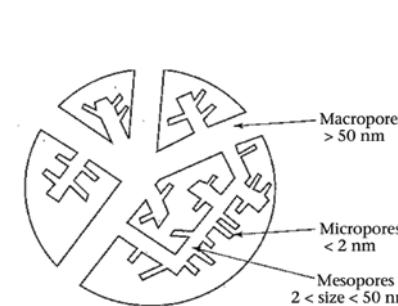


# Näiteid neutronhajumismeetodite rakendamisest

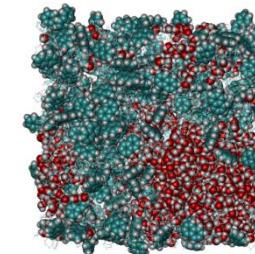
Dan Hüvonen  
*KBFI*



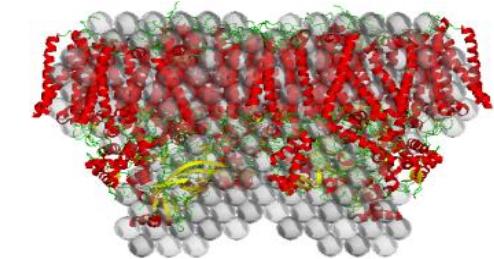
Tahkise füüsika  
ja magnetism



Füüsikaline keemia

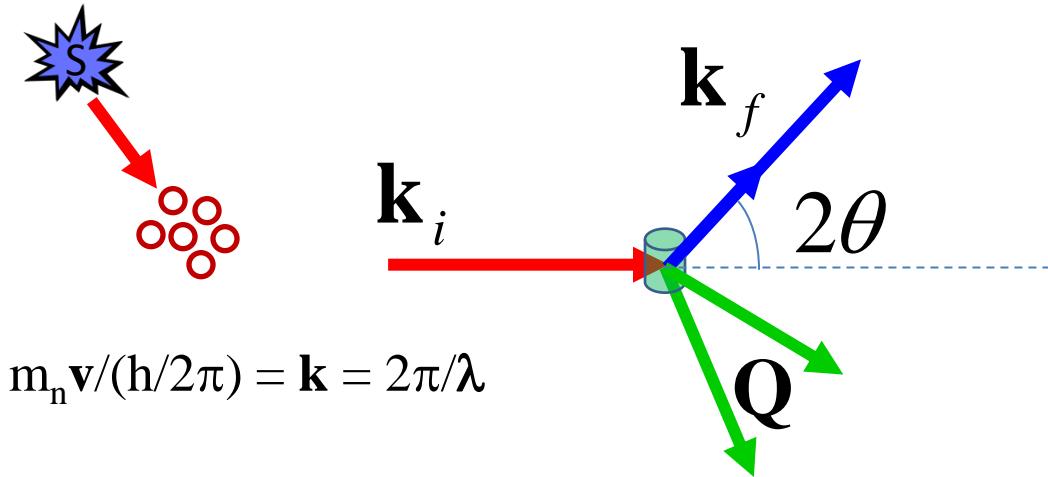


Orgaaniline  
keemia



Biofüüsika

# Neutronhajumine struktuur ja dünaamika



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

$$\hbar\omega = E_i - E_f$$

Braggi valem

$$n\lambda = 2d \sin \theta$$

Neutroni lainepikkus

Hajutajate vaheline  
kaugus aines

## Hajumine tuumadelt

$$S(\mathbf{Q}, \omega) = \frac{1}{2\pi\hbar} \int dt e^{-i\omega t} \frac{1}{N} \langle \rho_{\mathbf{Q}}(0) \rho_{-\mathbf{Q}}(t) \rangle$$

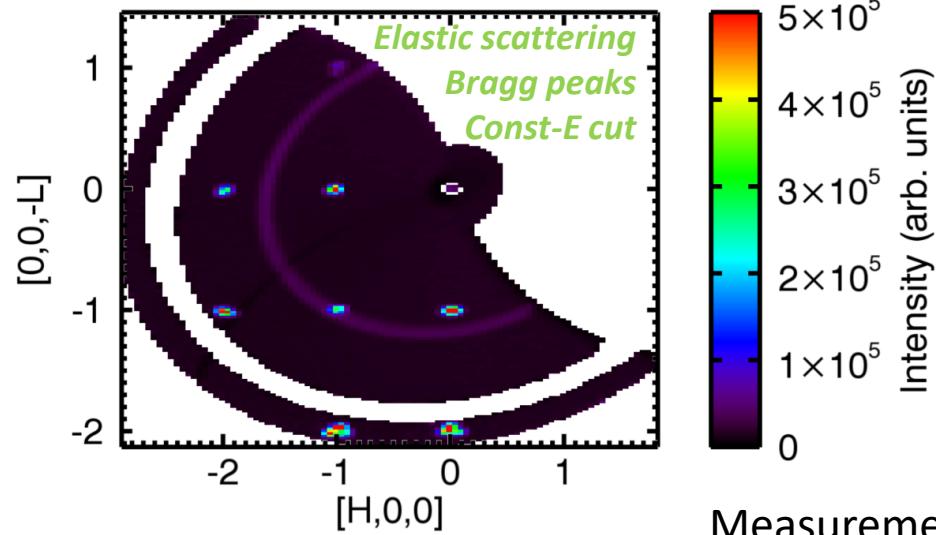
## Hajumine elektronide spinnidelt

$$S^{\alpha\beta}(\mathbf{Q}, \omega) = \frac{1}{2\pi\hbar} \int dt e^{-i\omega t} \frac{1}{N} \sum_{\mathbf{R}\mathbf{R}'} e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R}')} \langle S_{\mathbf{R}}^\alpha(0) S_{\mathbf{R}'}^\beta(t) \rangle$$

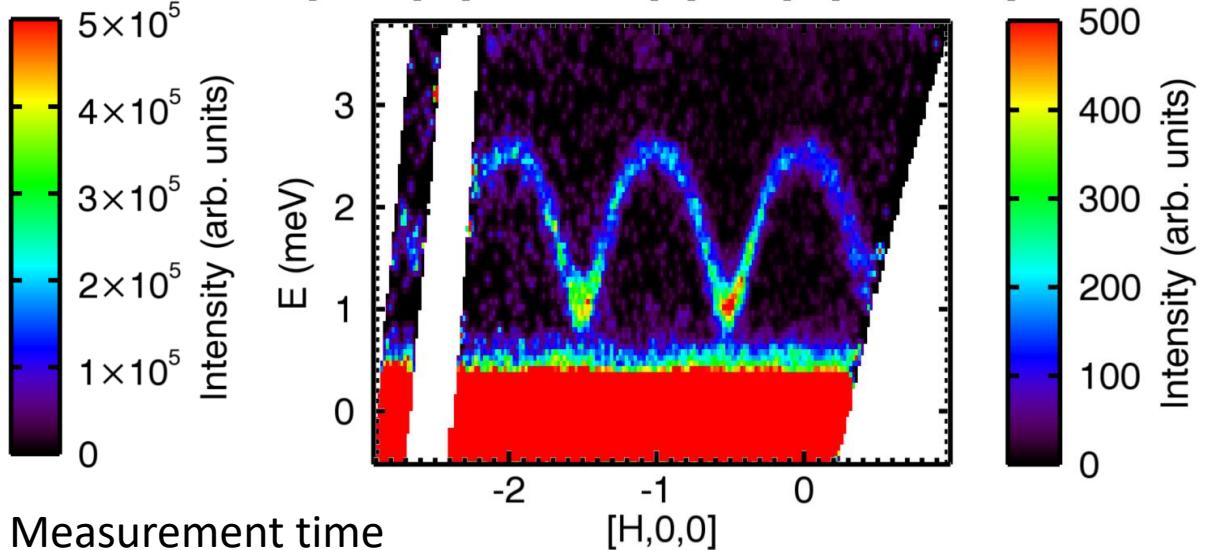
# Näide: neutronhajumise andmed

*lennuaja spktromeeter CNCS@ORNL*

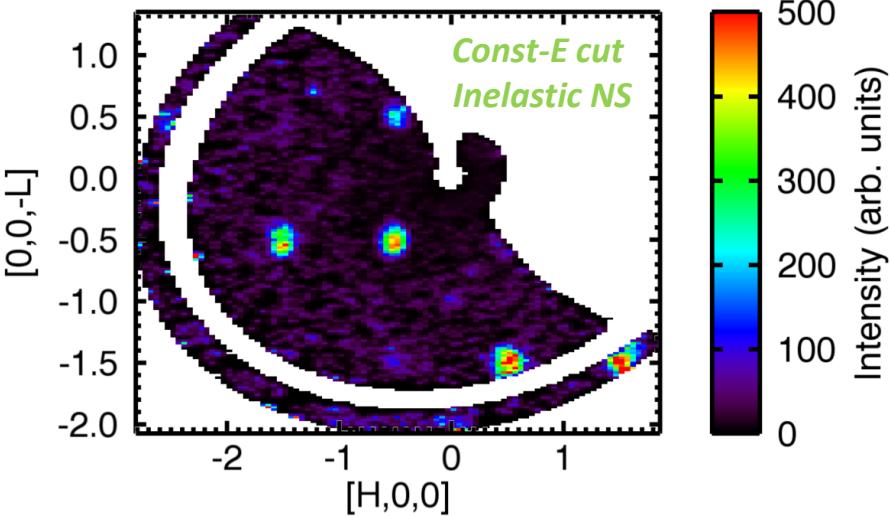
$E = [-0.2, 0.2]$  meV,  $[0, K, 0] = [-0.15, 0.15]$



$[0, 0, -L] = [-0.55, -0.45]$ ,  $[0, K, 0] = [-0.15, 0.15]$



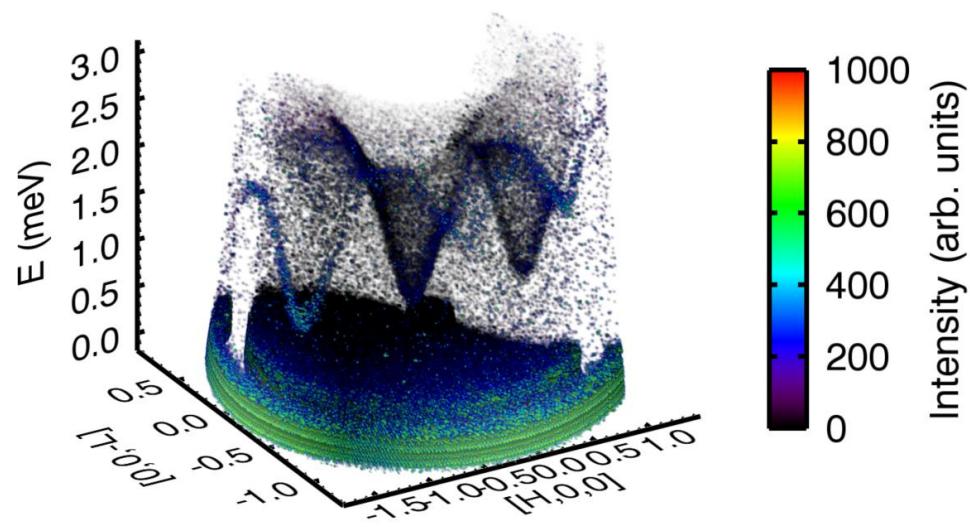
$E = [1, 1.2]$  meV,  $[0, K, 0] = [-0.15, 0.15]$



Measurement time

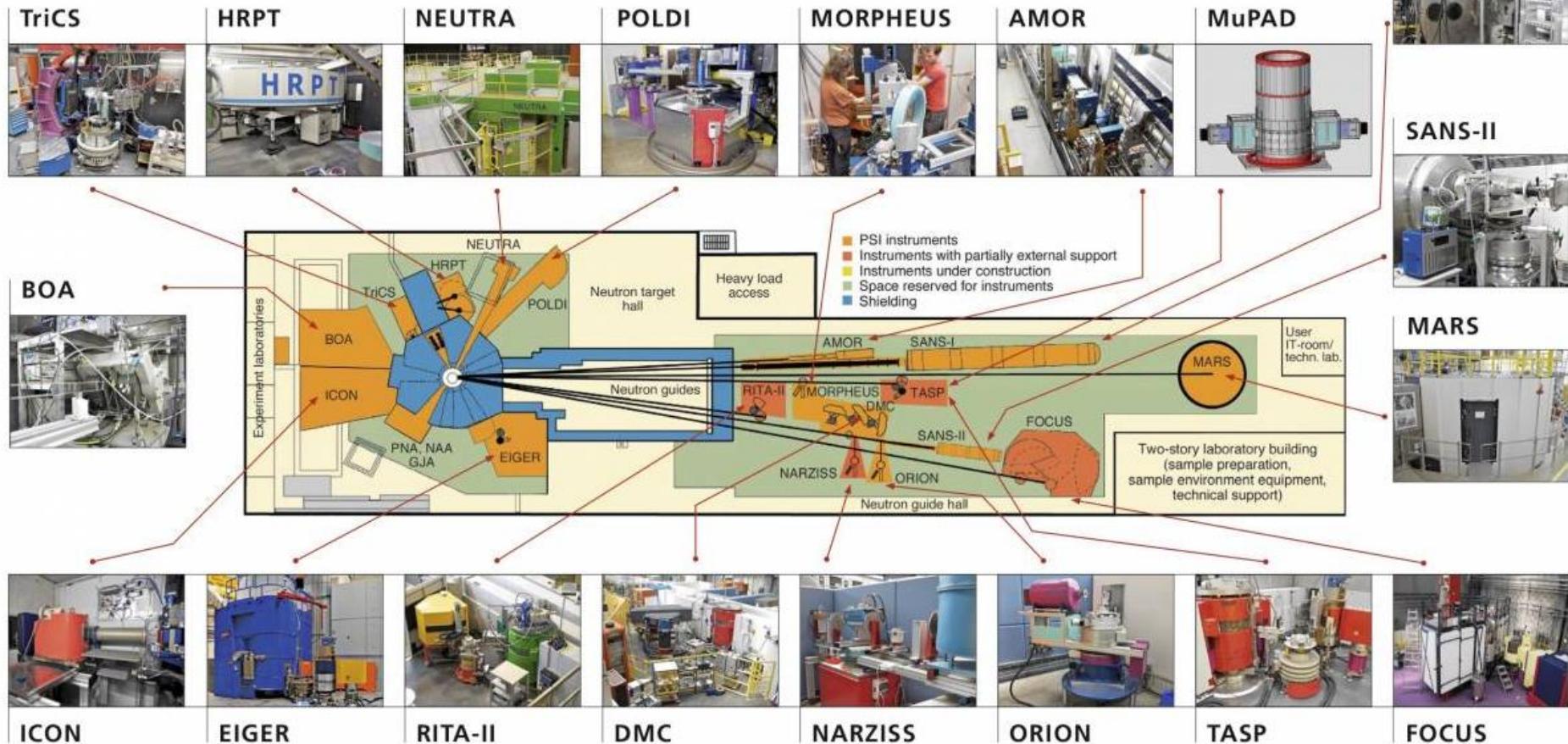
~30h

$[0, K, 0] = [-0.15, 0.15]$



# Neutronhajumise labor

## Neutron Scattering and Imaging Instruments at SINQ



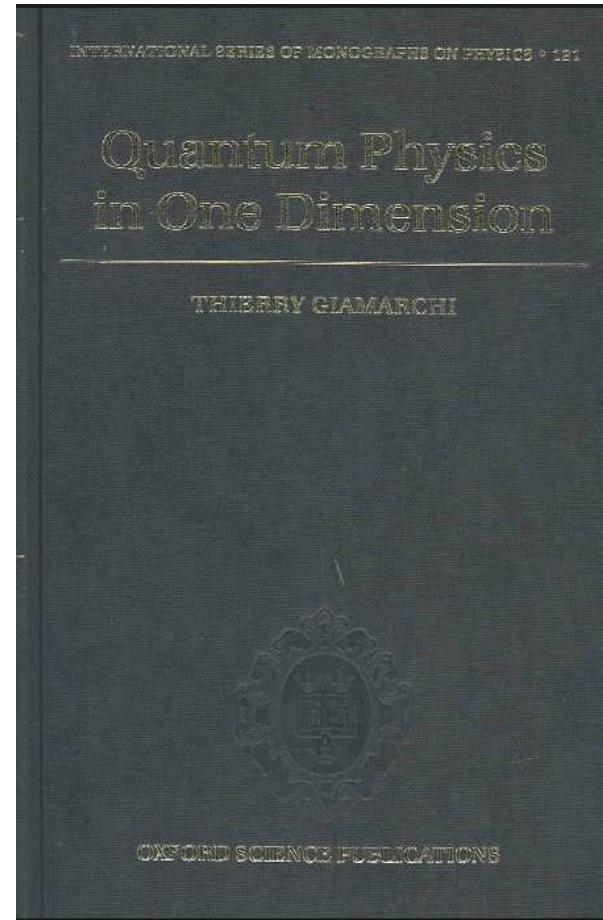
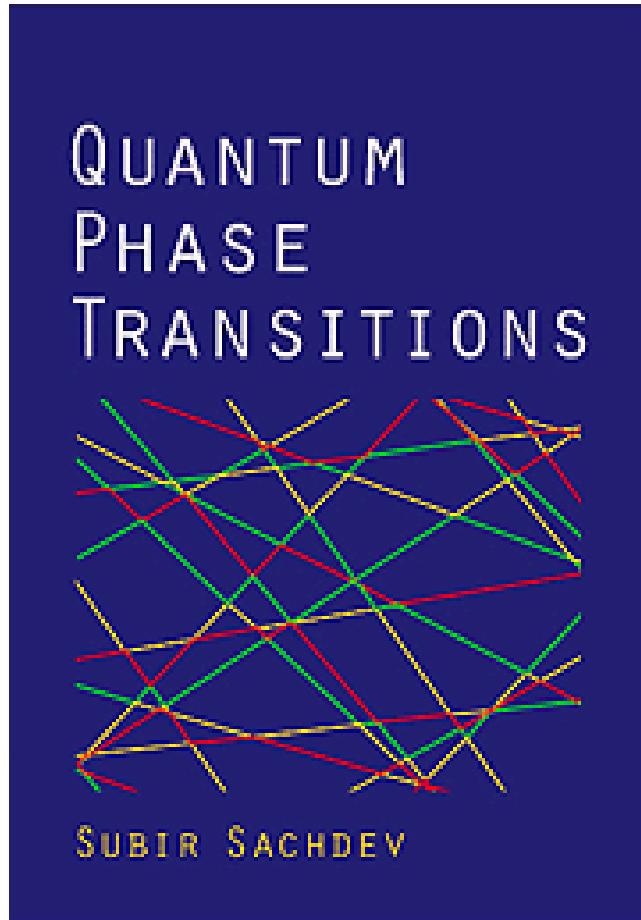
# Photos: D23@ILL with 12T magnet



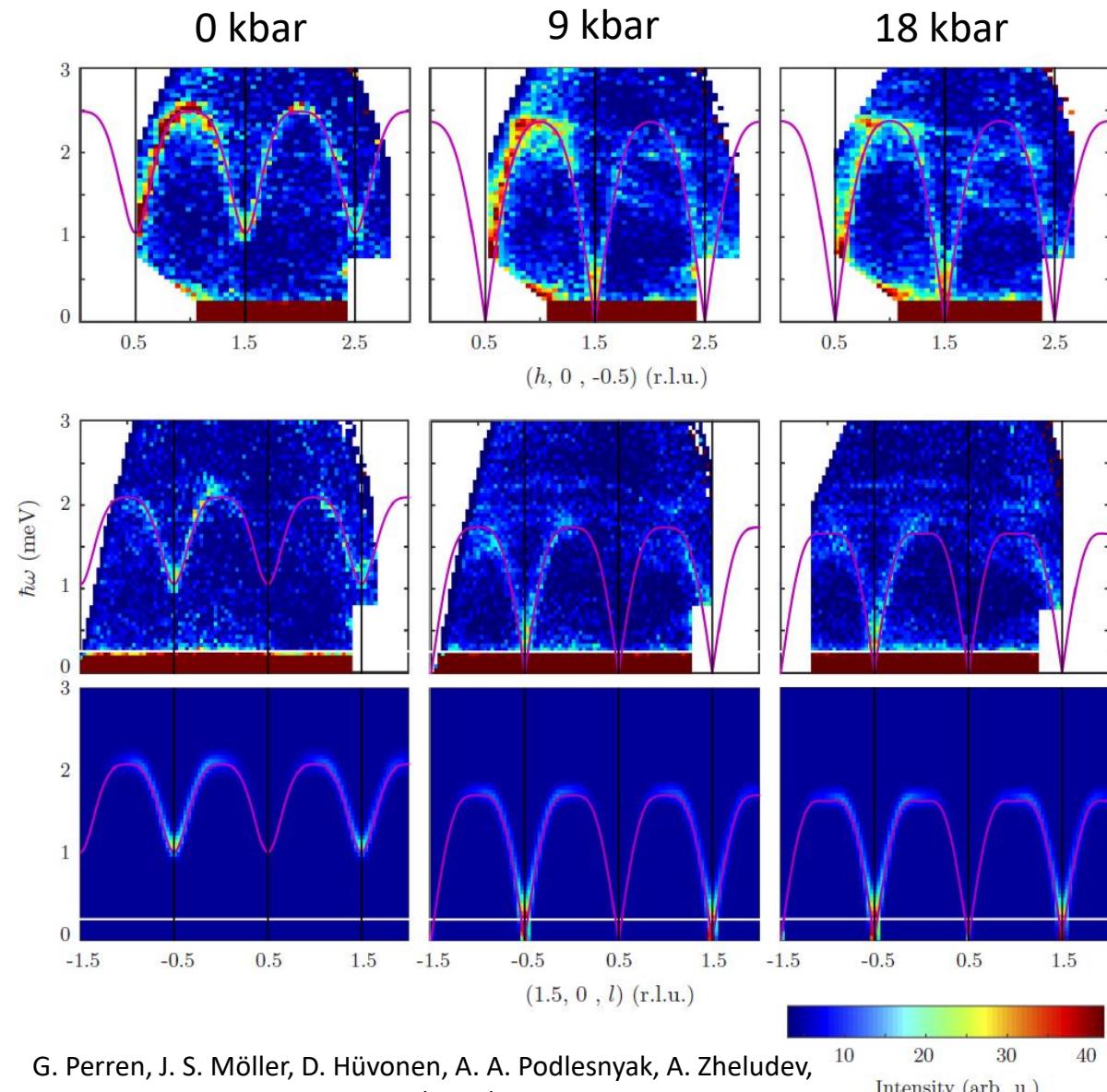
# Muudetavad eksperimentaalsed parameetrid

- Temperatuur (0.05 – 1800K)
- Magnetväli (0 – 15T)
- Elektriväli (0 - 5kV/L<sub>s</sub>)
- Rõhk (0 – 30000bar)
- In-situ reaktorid keemiliste ja bioloogiliste objektide jaoks

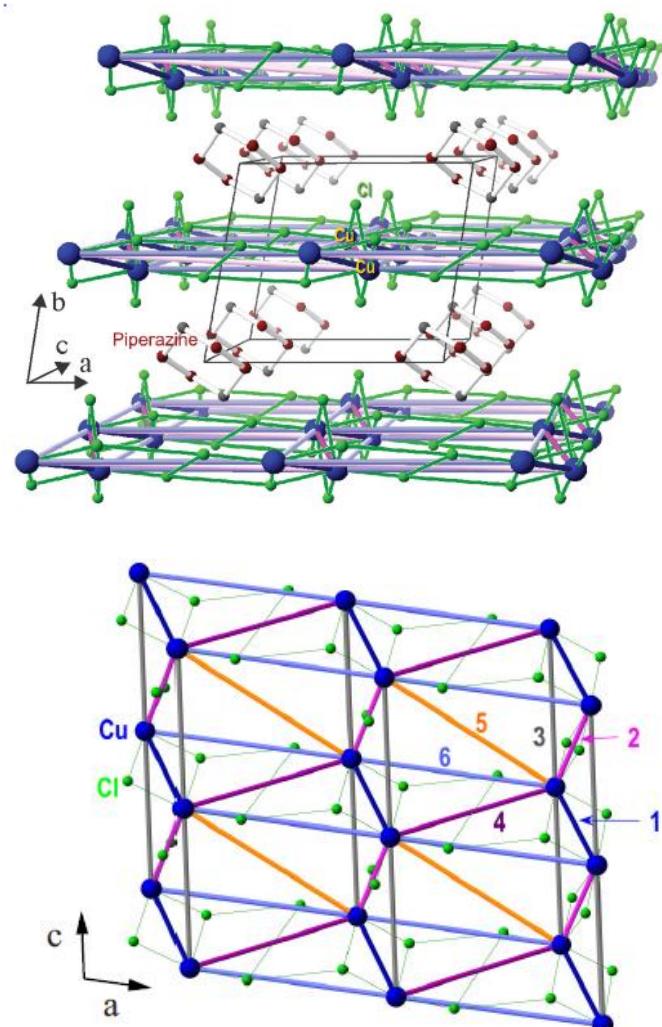
# Kvantfaasisiirded ja madaladimensionaalne füüsika



# Magnetiline korraстumine rõhu all



Spin dynamics in pressure-induced magnetically ordered phases in  $(C_4H_{12}N_2)Cu_2Cl_6$

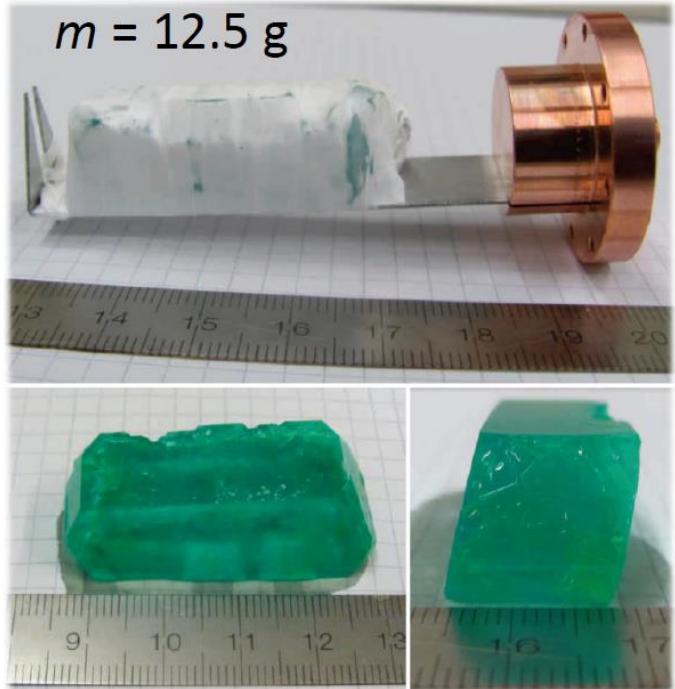
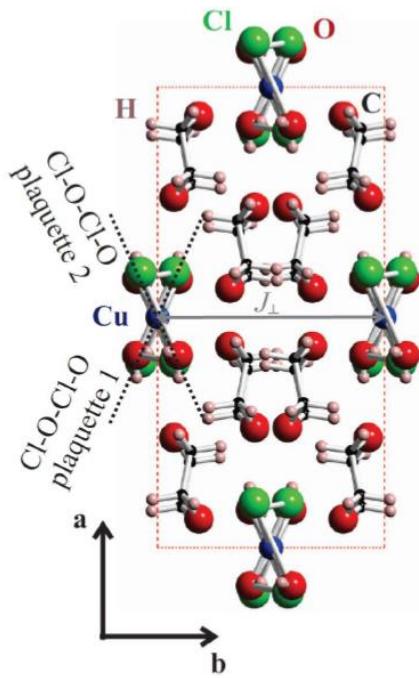
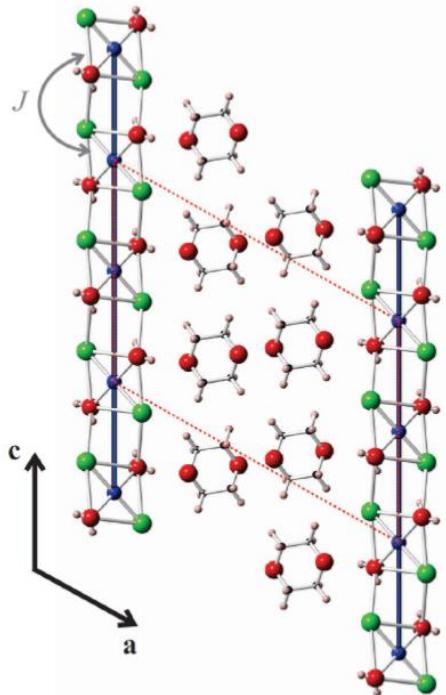


# Universality of 1D physics at T>0

## The Material: CuDCI

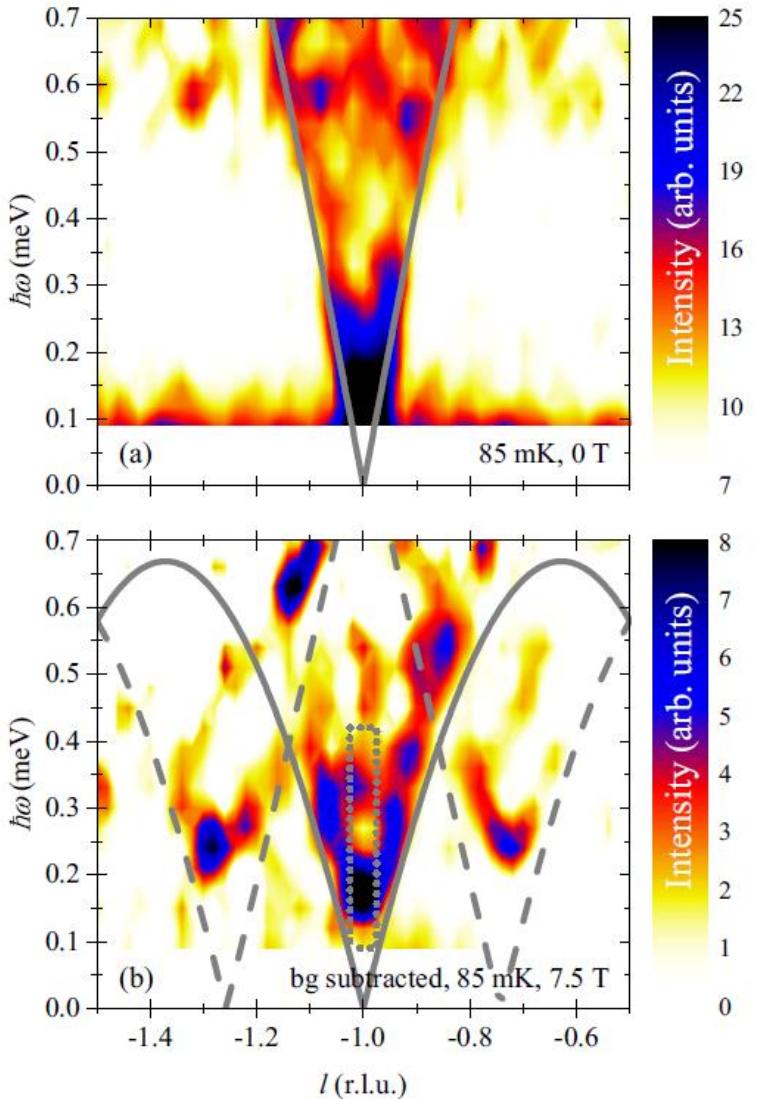
- $2(1,4\text{-Dioxane}) \cdot 2(\text{H}_2\text{O}) \cdot \text{CuCl}_2$
- Heisenberg  $S=1/2$  chain

- small staggered gyromagnetic tensor
- Tomonaga-Luttinger spin liquid (TLSL)



# Universality of 1D physics at T>0

- $T\chi''(\pi, \omega)$  is a universal function of  $\hbar\omega / k_B T$



## Luttinger spin liquid: Haldane's conjecture

istic of a larger universality class of systems, which includes most, and probably all, 1D fermi-  
on systems with a gapless linear spectrum. By



- All low-energy properties are a universal functions of  $v_F$  and  $K$
- All 1D magnets with a gapless linear spectrum are like that!

Among the physical systems believed to be described by the Luttinger model are:

- artificial 'quantum wires' (one-dimensional strips of electrons) defined by applying gate voltages to a two-dimensional electron gas, or by other means (lithography, AFM, etc.)
- electrons in carbon nanotubes
- electrons moving along edge states in the fractional Quantum Hall Effect
- electrons hopping along one-dimensional chains of molecules (e.g. certain organic molecular crystals)
- fermionic atoms in quasi-one-dimensional atomic traps
- a 1D 'chain' of half-odd-integer spins described by the Heisenberg model (the Luttinger liquid model also works for integer spins if they are in a large enough magnetic field)

# Scaling for partially magnetized CuDCl

scaling form [5]:  $S(\pi, \omega) = T^{-\alpha} \Phi\left(\frac{\omega}{T}\right)$

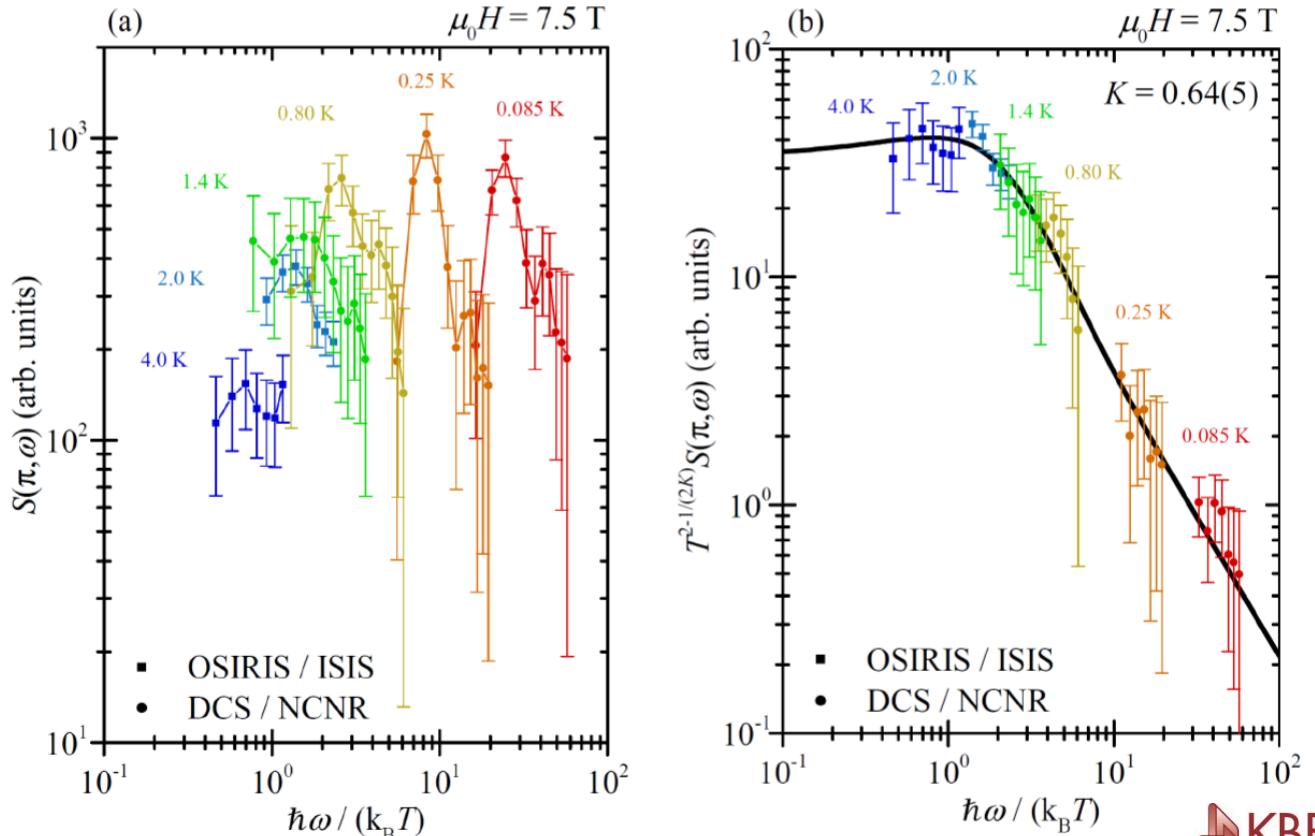
TLNL [6]:  $\alpha = 2 - \frac{1}{2K}$ ,  $\Phi\left(\frac{\omega}{T}\right) \propto \left( \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} + 1 \right) \text{Im} \left[ \left( \frac{\Gamma\left(\frac{1}{8K} - i\frac{\hbar\omega}{4\pi k_B T}\right) \Gamma\left(1 - \frac{1}{4K}\right)}{\Gamma\left(1 - \frac{1}{8K} - i\frac{\hbar\omega}{4\pi k_B T}\right)} \right)^2 \right]$

restrictions:

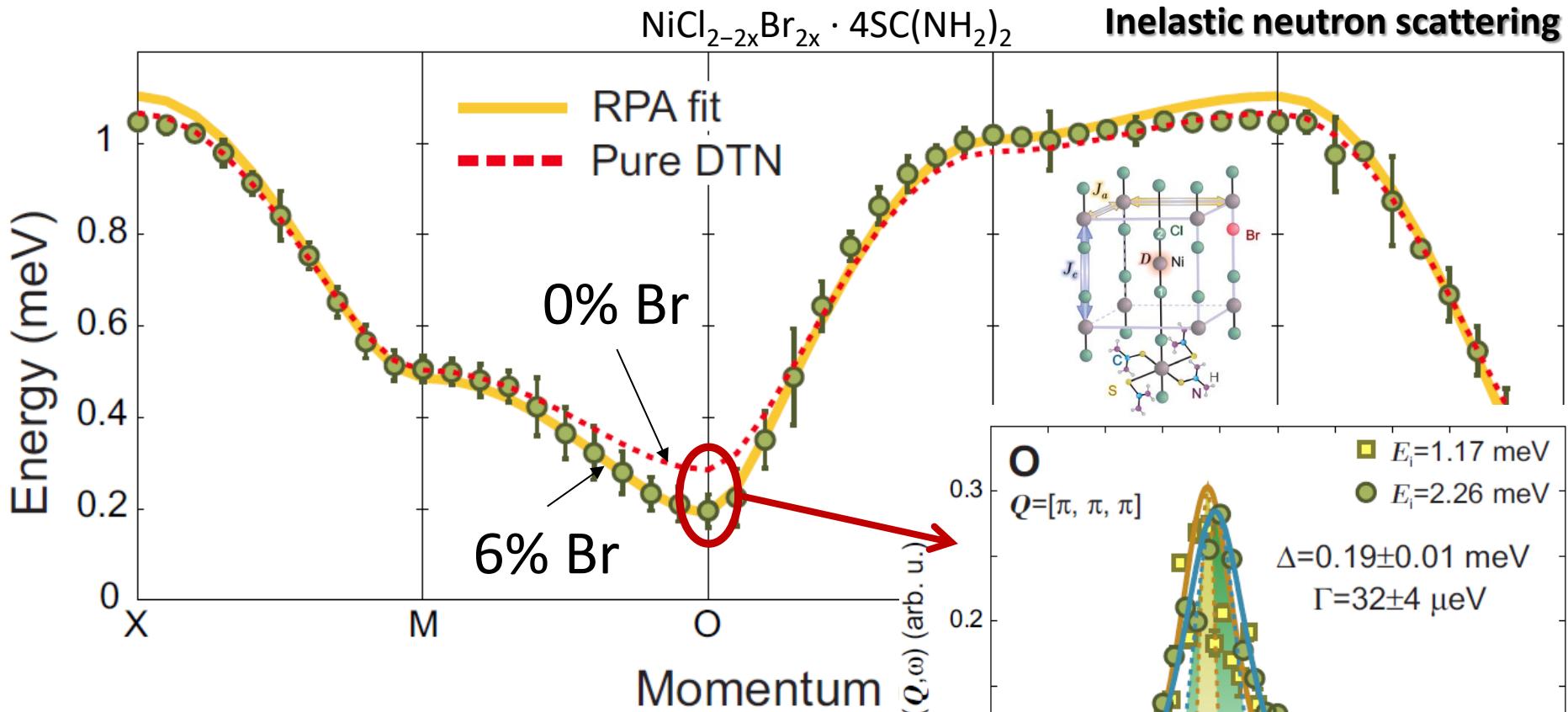
*energy gap*  
 $(T \geq 2.8 \text{ K})$  or  
 $(\hbar\omega \geq 0.24 \text{ meV})$

*longitudinal correl.*  
*and non-linear regime*

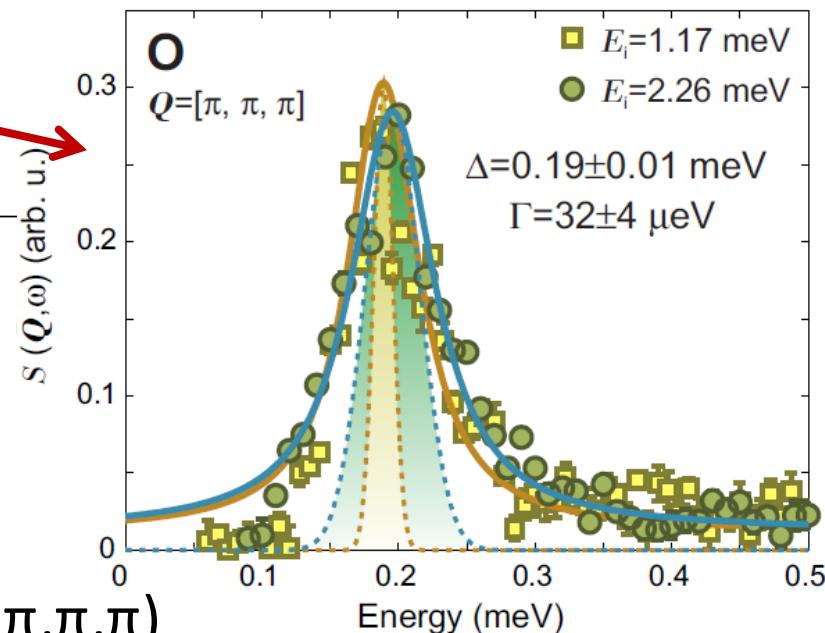
$k_B T, \hbar\omega \lesssim 0.4 \text{ meV}$



# Korrapäratusega kvantmagnet



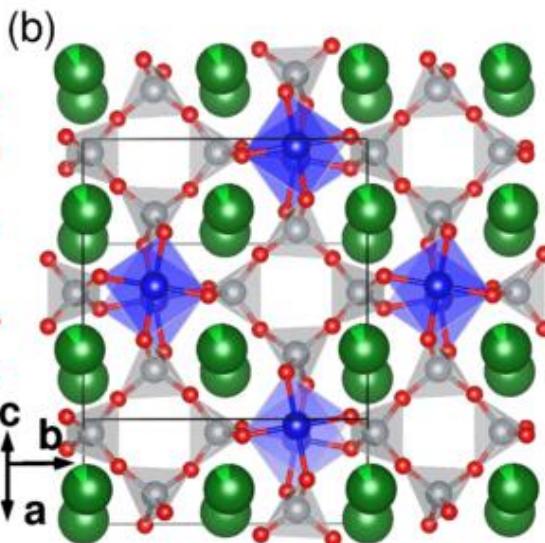
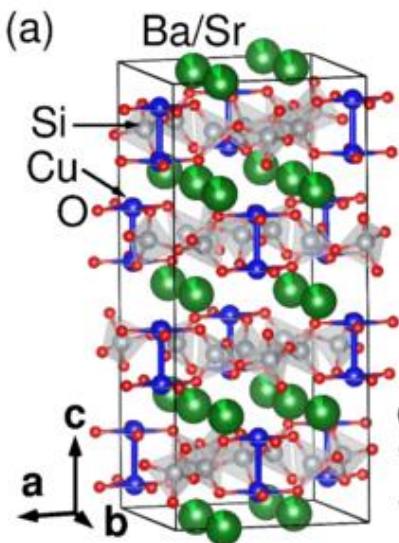
Inelastic neutron scattering



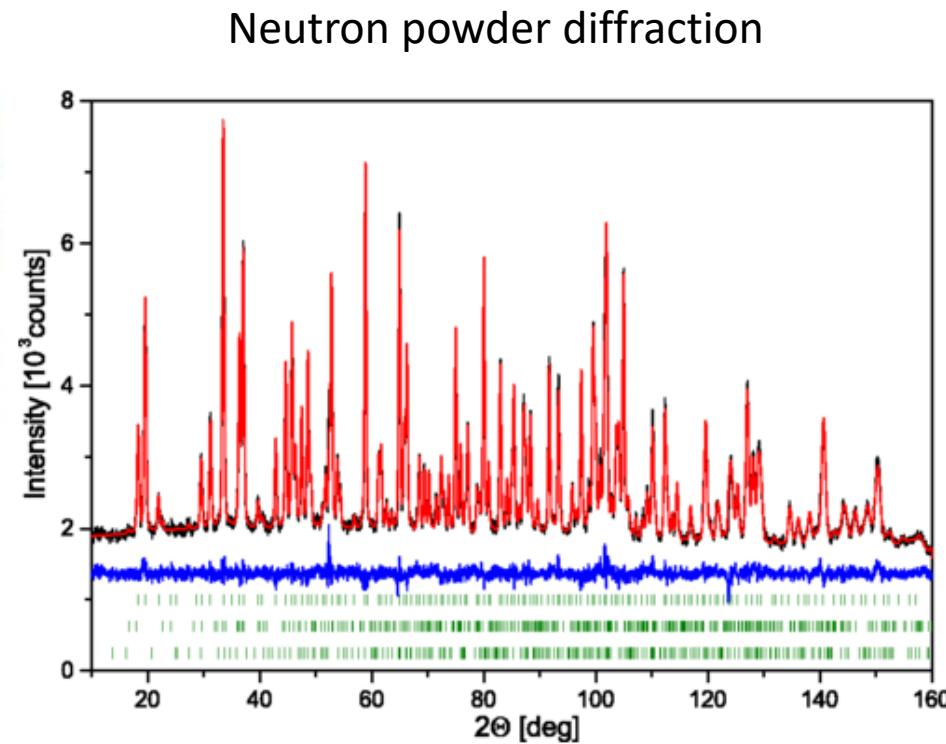
With bond disorder:

- ✓ Gap reduces ( $D$ )
- ✓ Bandwidth increases ( $J_c$ )
- ✓ Magnon lifetime reduces most at  $Q=(\pi,\pi,\pi)$

# Stabilization of the tetragonal structure in $(\text{Ba}_{1-x}\text{Sr}_x)\text{CuSi}_2\text{O}_6$

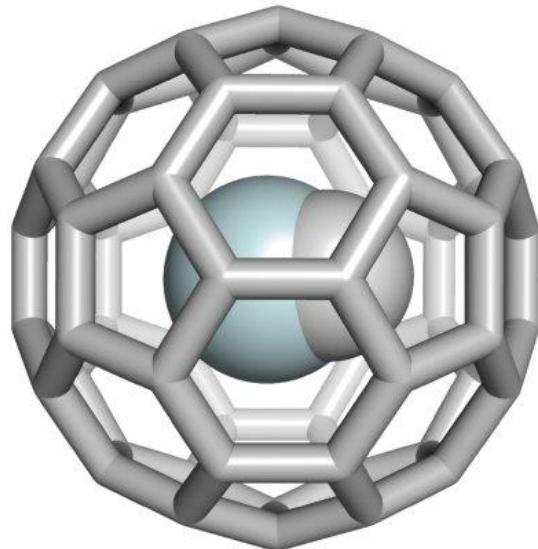


Interesting Quantum Magnetic model system

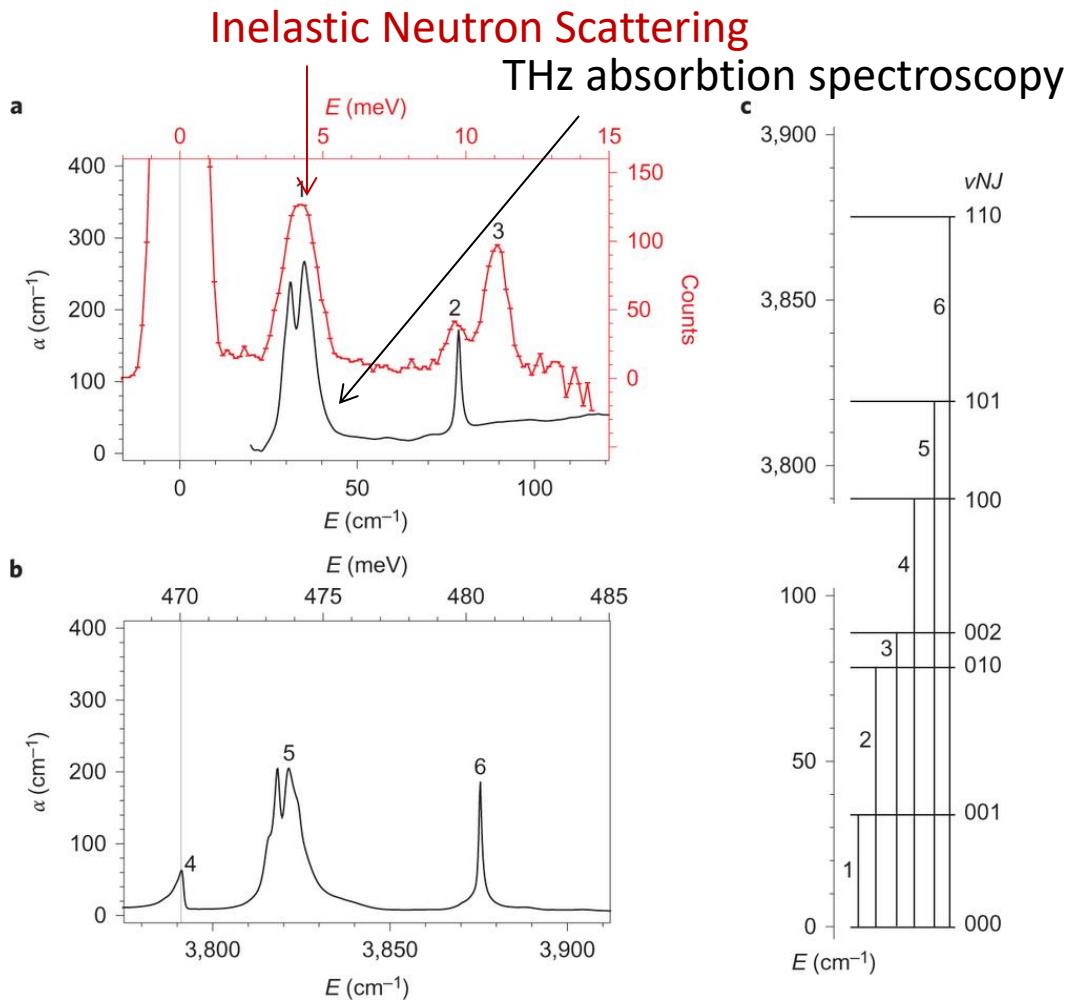


P. Puphal, D. Sheptyakov, I. Heinmaa, R. Stern, et al. *Phys. Rev. B* **93**, 174121 (2016)

# The dipolar endofullerene HF@C<sub>60</sub>

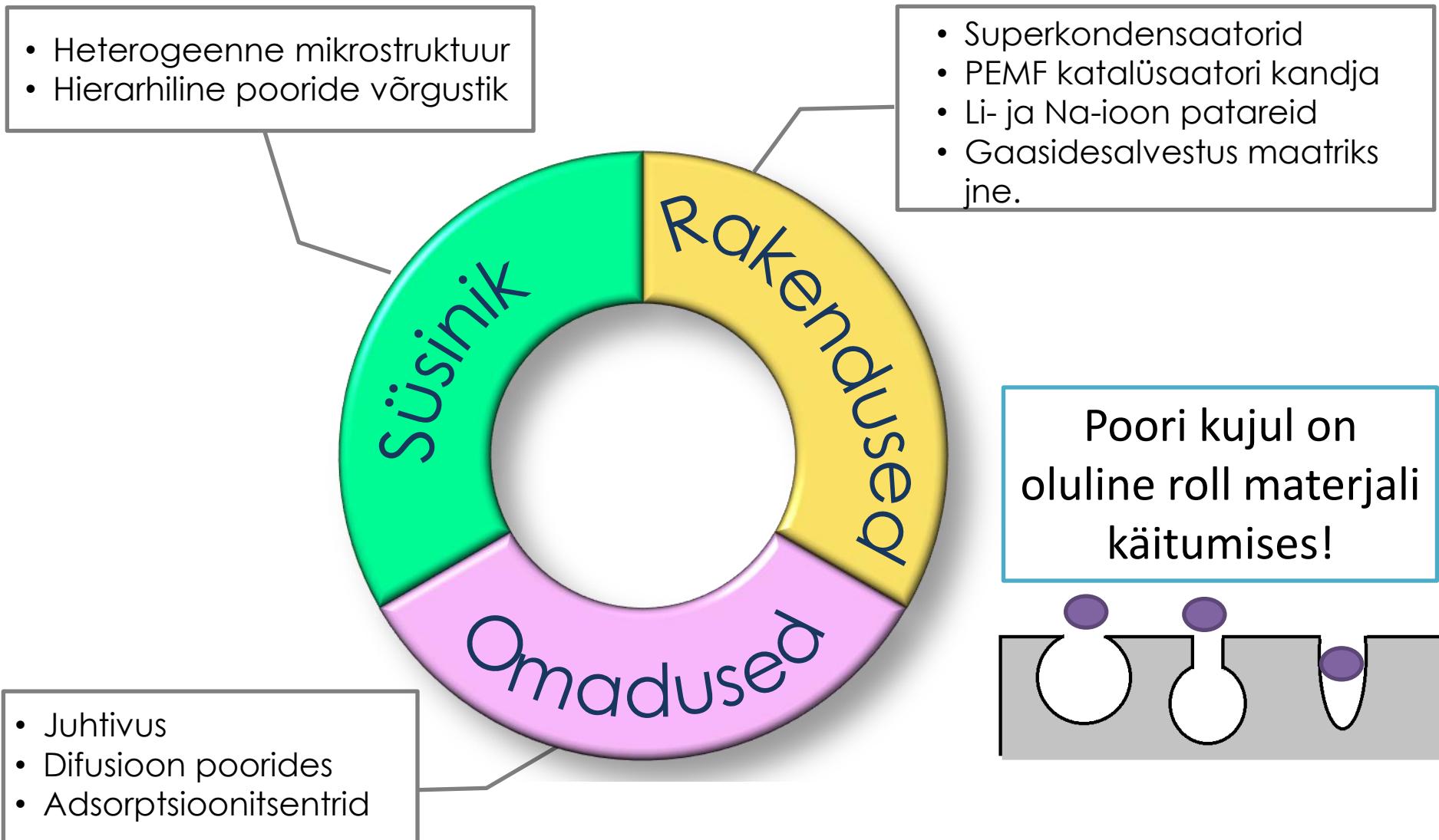


HF@C<sub>60</sub>

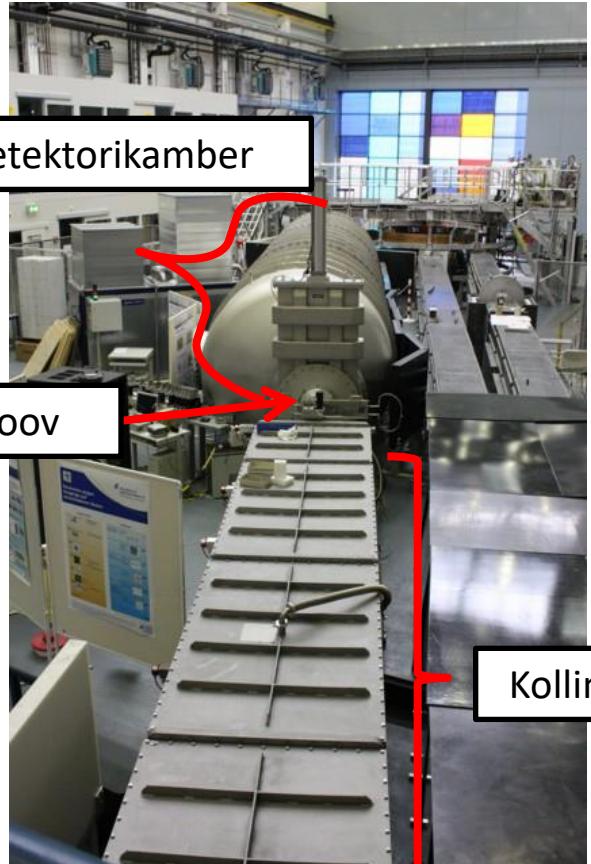


Krachmalnicoff A, Bounds R, Mamone S, Alom S, Concistrè M, Meier B, Kouřil K, Light ME, Johnson MR, Rols S, Horsewill AJ, **Shugai A, Nagel U, Rõõm T**, Carravetta M, Levitt MH, Whitby RJ, *Nature Chemistry* 8, 953–957 (2016)

# Mikropoorsed süsinikmaterjalid

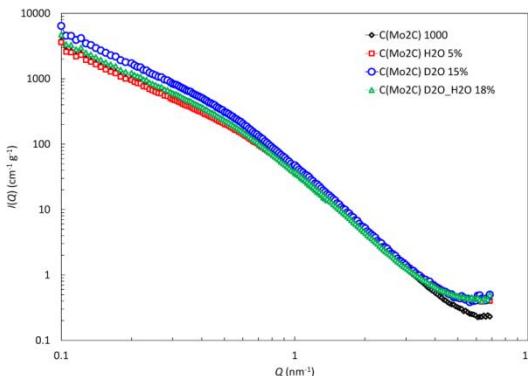
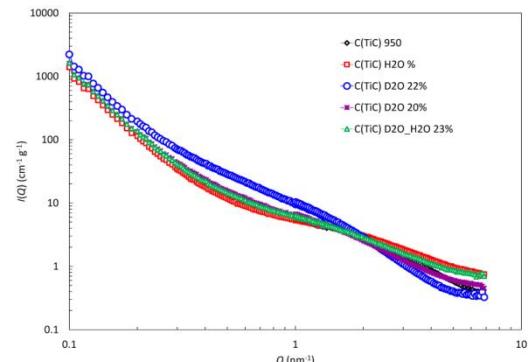
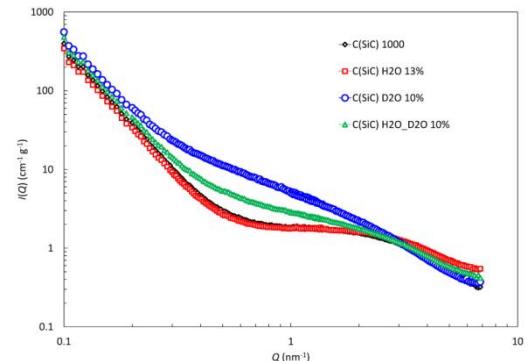


# Väikese nurga all neutronhajumine - SANS



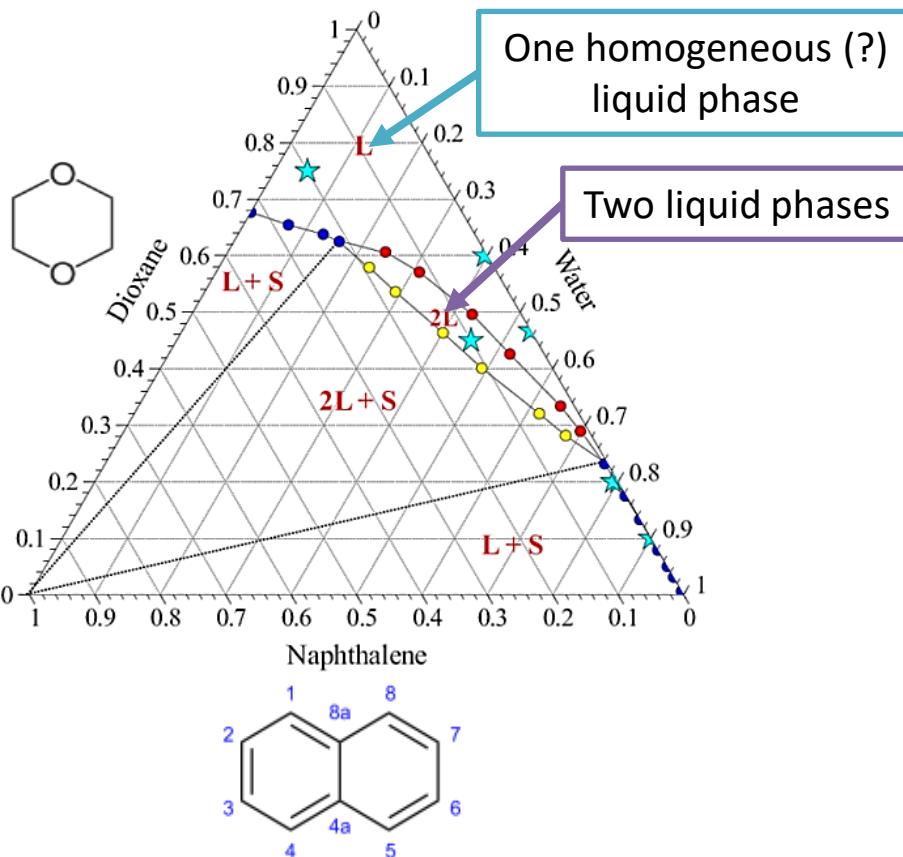
SANS  
Elastne neutronite  
hajumine

Berlin HZB V16:  
TOF  
 $0.25 \text{ nm} < \lambda < 1.8 \text{ nm}$   
 $0.001 \text{ nm}^{-1} < Q < 8.0 \text{ nm}^{-1}$   
i.e.  $6300 \text{ nm} > \lambda > 0.78 \text{ nm}$



# Microheterogeneity in homogeneous liquid mixtures – key to understanding solubility and phase separation

Three-component phase diagram for the mixture of 1,4-dioxane, naphthalene, and water



1,4-dioxane is widely used as solvent

- Fully mixable with water
- Suitable for processes with varying water content
- Also at industrial scale

Adding naphthalene causes phase separation ↙

- Not in other organic solvents fully mixable with water

## An unique behaviour!

Understanding the microheterogeneity in such mixtures helps to understand the reasons for phase separation and use it in various applications for better outcome!

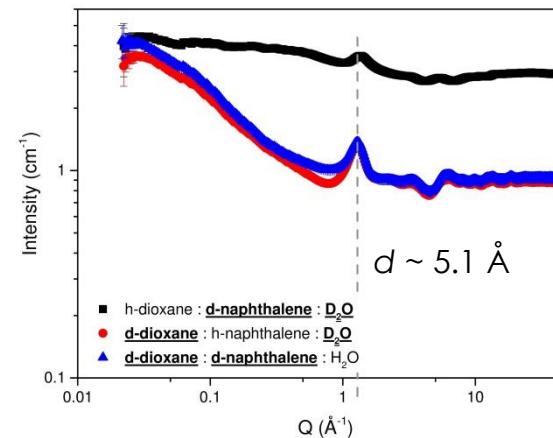
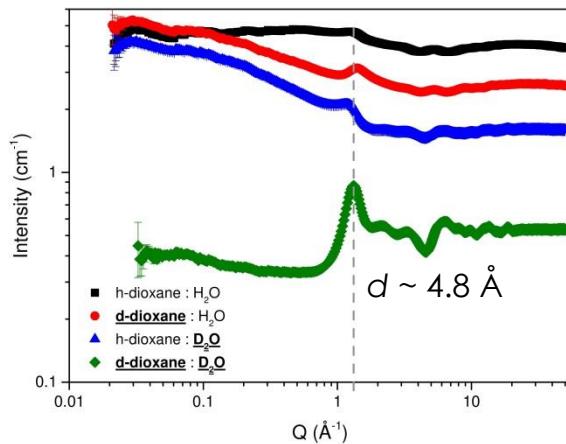
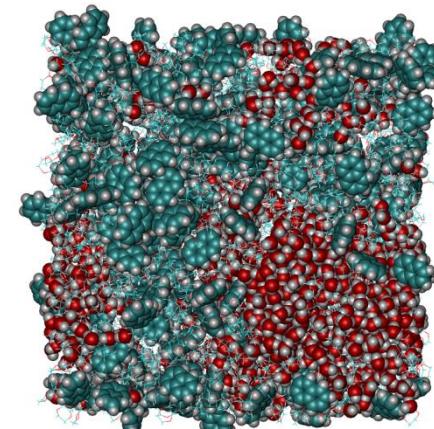
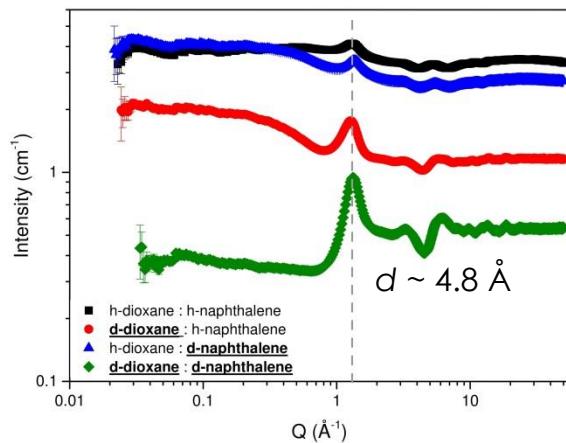
## Possible applications

- Complex tuning of reaction environment
  - Optimizing phase separation at the industrial scale
  - Avoiding phase separation when needed
- Etc.

O. Kekšev, S. Salmar et.al 2016, personal communication  
Measurements carried out @ NIMROD, RAL, ISIS, Didcot, UK

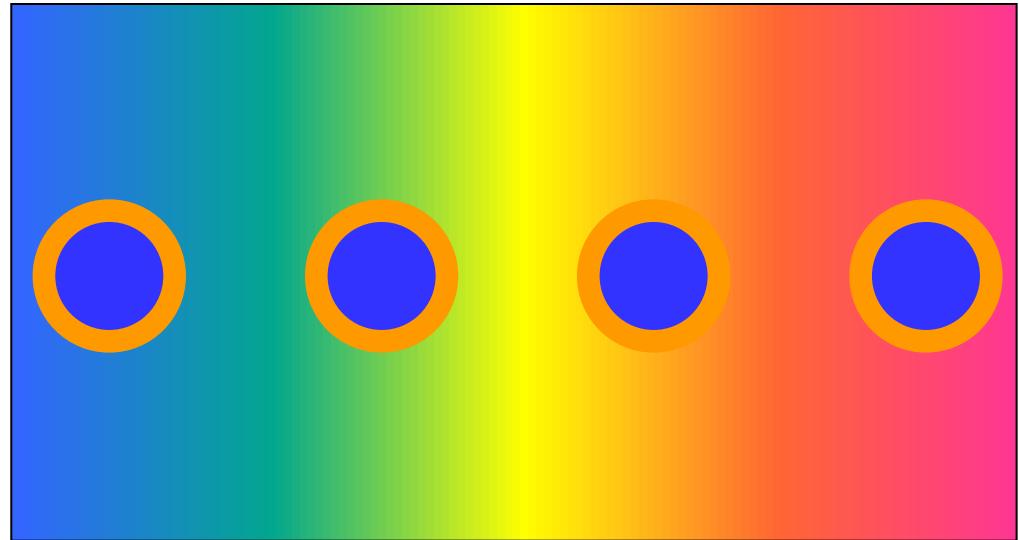
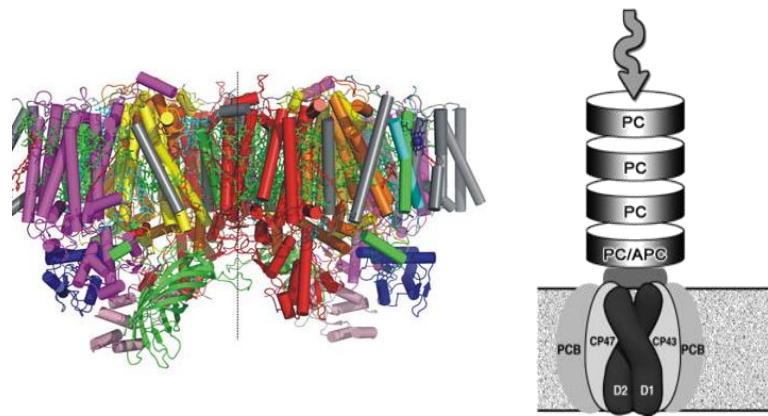
# Microheterogeneity in homogeneous liquid mixtures – key to understanding solubility and phase separation

1,4-dioxane, napthalene, and water



O. Kekšev, S. Salmar et.al 2016, personal communication  
Measurements carried out @ NIMROD, RAL, ISIS, Didcot, UK

# Small Angle Neutron Scattering

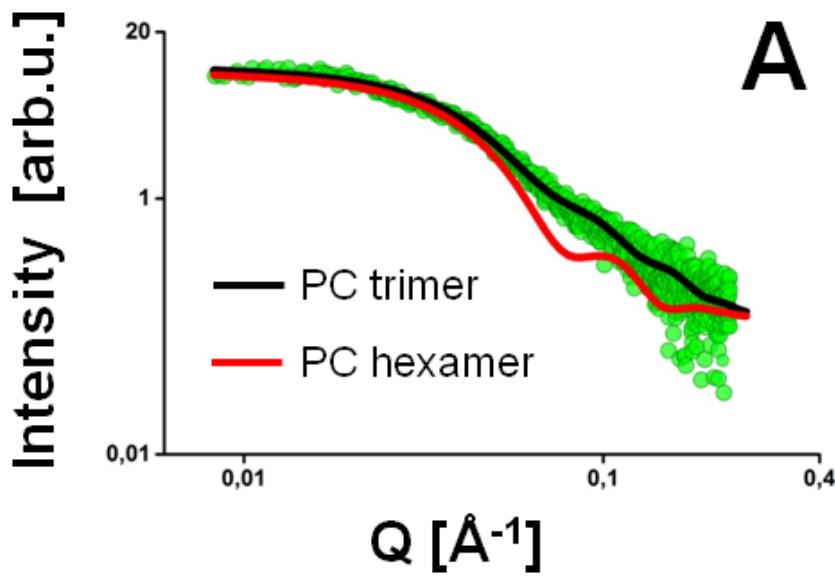


SANS provides: low-resolution structures (**only**), but:

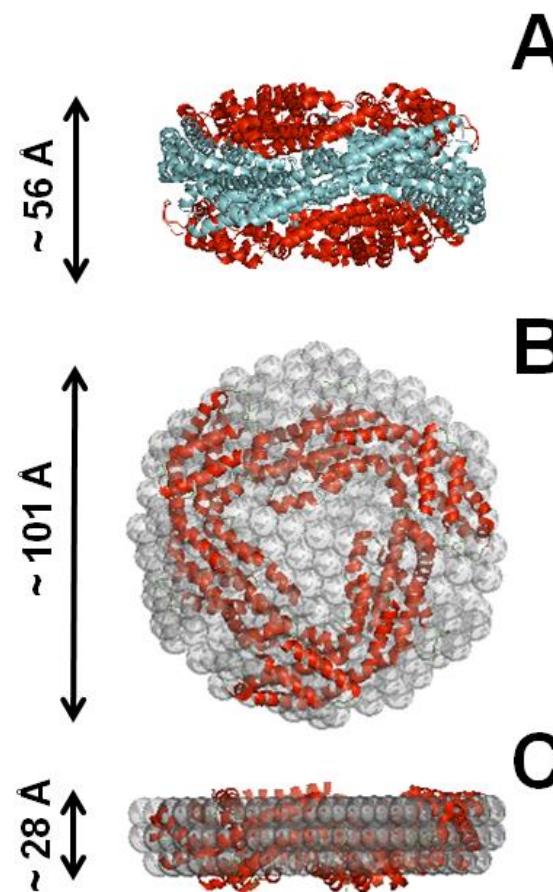
- → **structure at close to in-vivo conditions**
- possible at room temperature
- **contrast variation** yields protein and detergent shell separately

Nagy, G., Garab, G., and Pieper, J. (2014) in:  
Contemporary Problems of Photosynthesis (Editors: S.  
Allakhverdiev, A. B. Rubin, V. A. Shuvalov)

# Solution Structures from SANS/SAXS

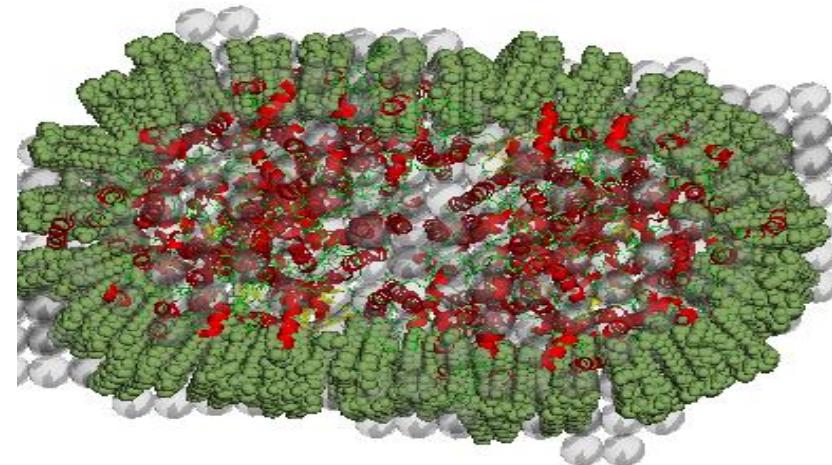
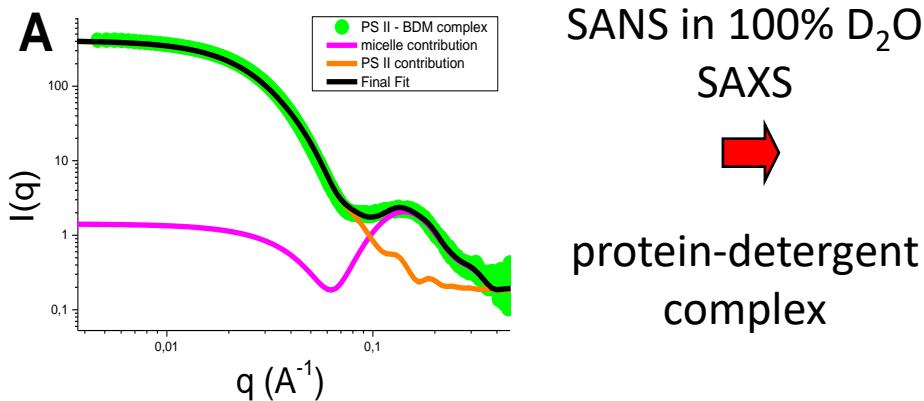
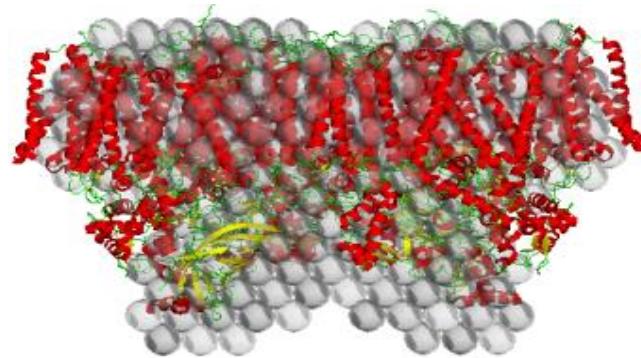
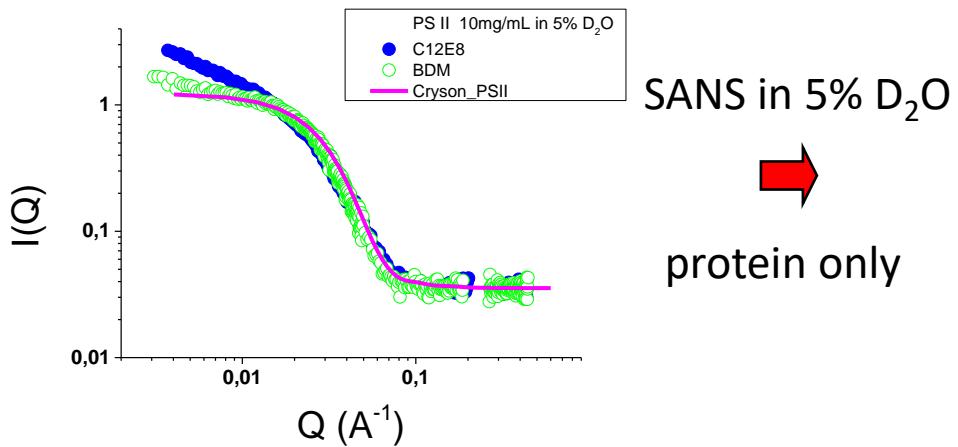


SAXS  
→



→ Determination of protein structure in solution

# Solution Structures from SANS/SAXS



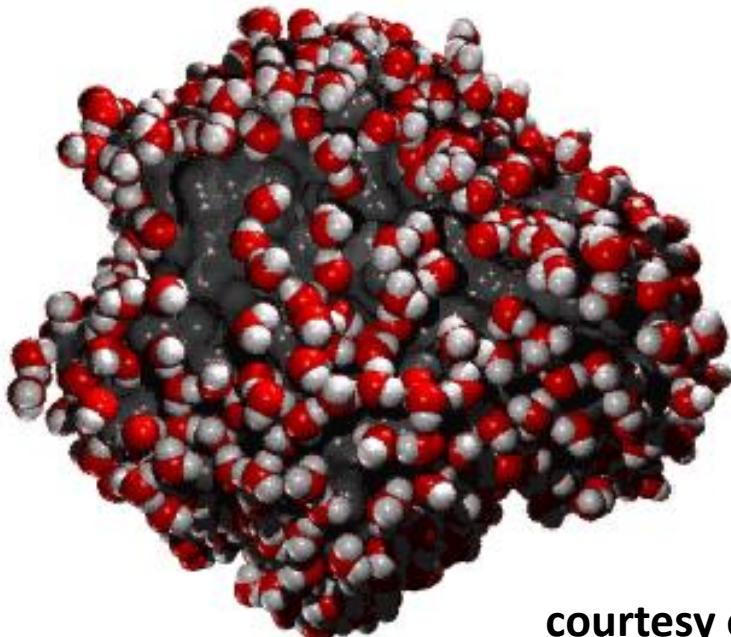
→ Solution structure compares well to PSII X-ray structure  
Detergent belt from contrast variation

# Neutron Spectroscopy

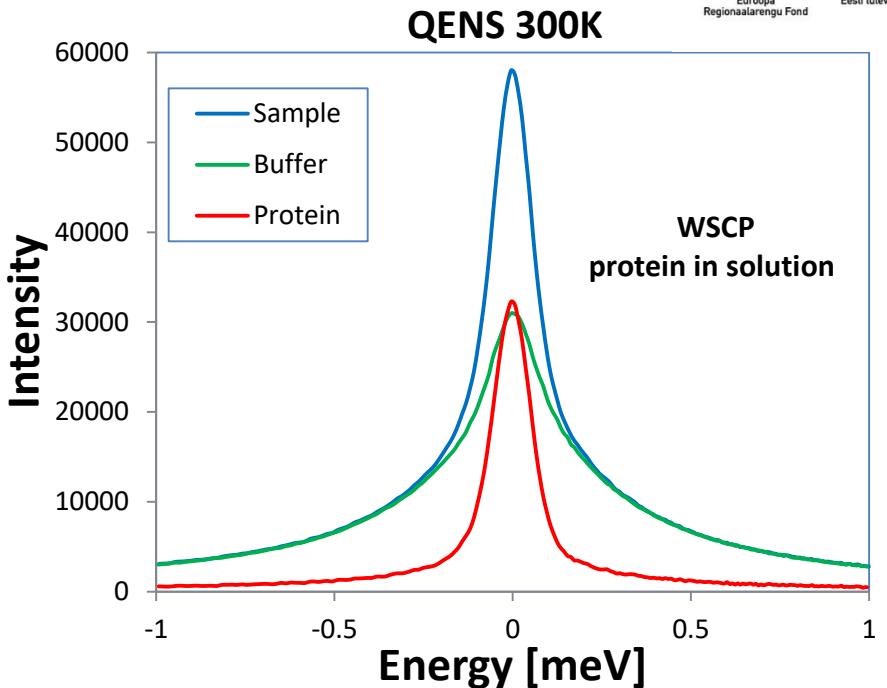
## (QENS - quasielastic neutron scattering)

Incoherent scattering function  $S(Q, \omega)$ :

$$S_{inc}(\vec{Q}, \omega) = \frac{1}{2\pi} \cdot \int_{-\infty}^{\infty} e^{-iat} \int_{-\infty}^{\infty} e^{i\vec{Q}\vec{r}} \cdot G_s(\vec{r}, t) d\vec{r} dt$$



courtesy of  
Prof. D.Tobias



**QENS measures water and protein motions via energy and momentum exchange**

**Motions seen are: diffusion, local reorientations, vibrations, phonons**

**Applications: protein/water dynamics  
Phase transitions, hydrogen storage**

# Kokkuvõte

- Neutronhajumine on kasulik laia haardega uurimismeetod.
- Neutronhajumismeetodite kvaliteet ja kasutajasõbralikkus suurenevad pidevalt
- Eestist võiks rohkem kasutajaid olla!  
Võtke julgelt ühendust!

