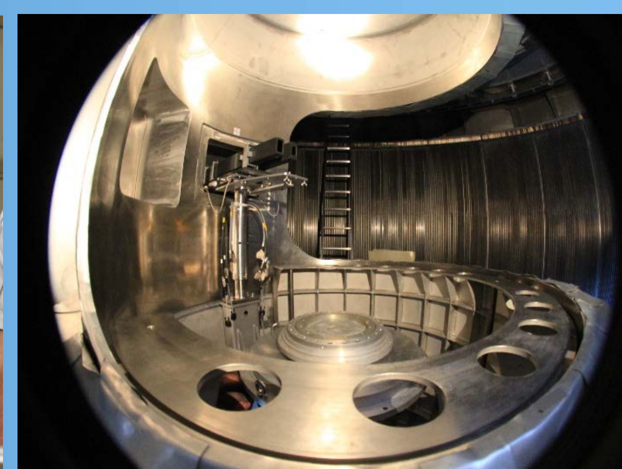
New neutron spectrometer NEAT at HZB:

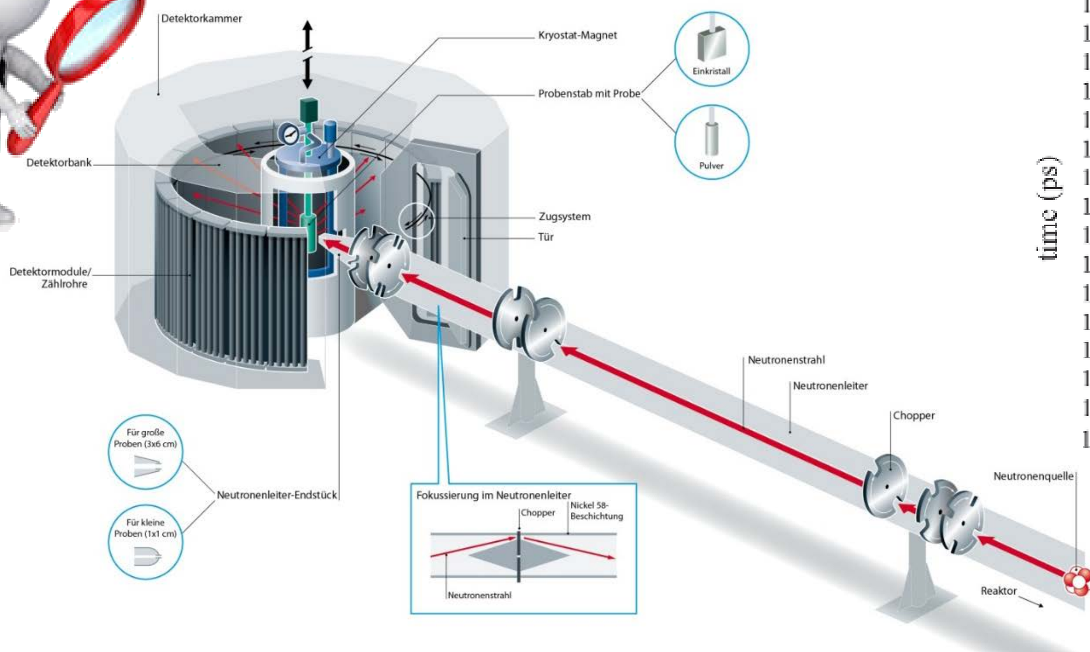
experience from one year of user operation

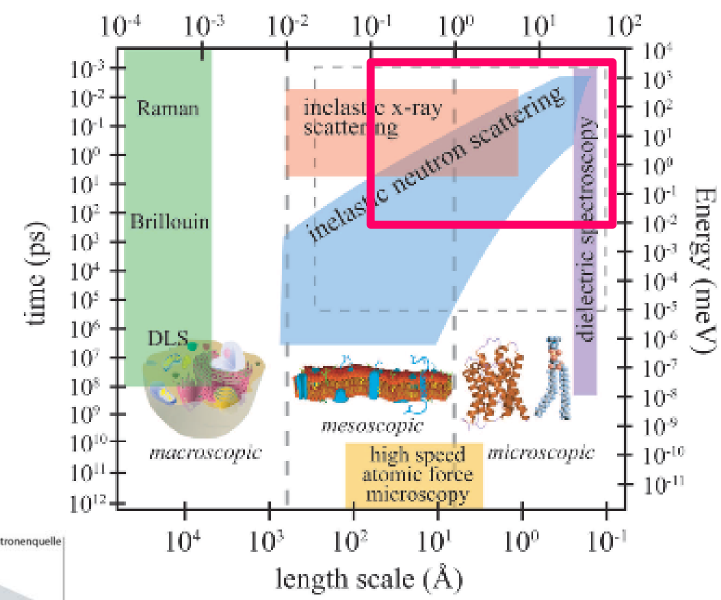
Margarita Russina



HZB Helmholtz Zentrum Berlin

Spectrometer NEAT@Helmholtz Zentrum Berlin





J. Cardiovasc. Dev. Dis. 2015, 2, 125-140c

Simultaneous access to the broad time and length scales important for nanomaterials:

Time scale: $10^{-14} \div 10^{-10}$ s

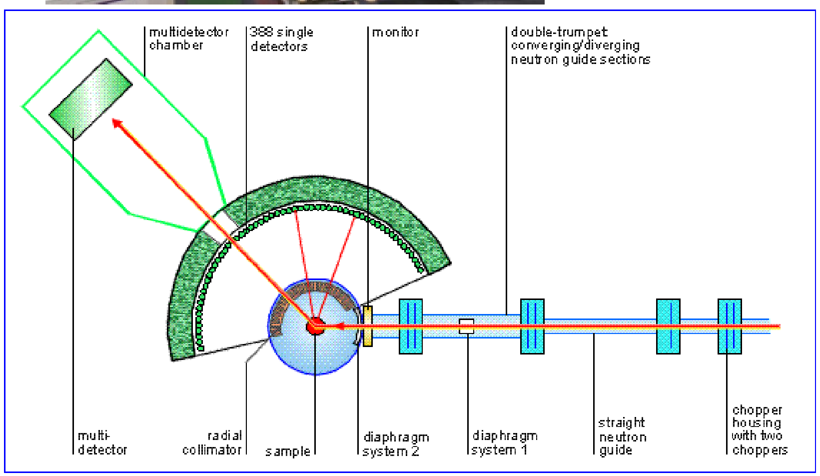
Length scale: 0.5-100 Å

Broad range of sample environment: T= 40 mK ÷ 1000 K

Operation since 1995, upgrade in 2010-2016

NEAT'1995

- Operation since 1995, work-horse instrument
- Science: fast diffusion and low energy excitations in broad range of materials (not single X-talls)
- Focus: microscopic dynamics in disordered and crystalline powder samples



V3

Instrument characteristics:

-Flexible chopper speed, wide range of resolution, wide accessible wavelength range

-High (1000° C) and low (mK) temperatures

-Primary flight path 13.2 m; secondary flight path 2.5 m

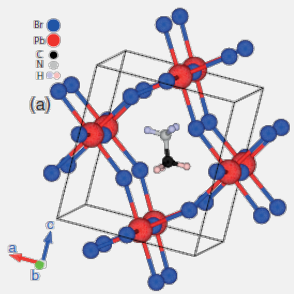
"Zero cost" improvements in 2004-2005:

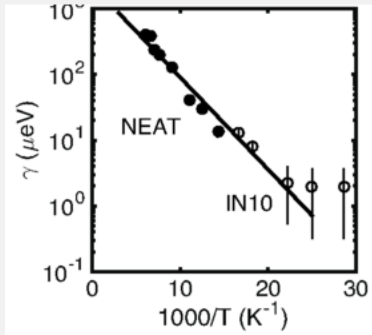
-Increase of intensity by factor of 2-4 due to the implementation of the trapezoidal chopper pulse shape

-Increase of the useful wavelength range by utilization of the short wavelength neutrons

-Implementation of the magnetic field up to 5T and in-situ H_2 gas pressure

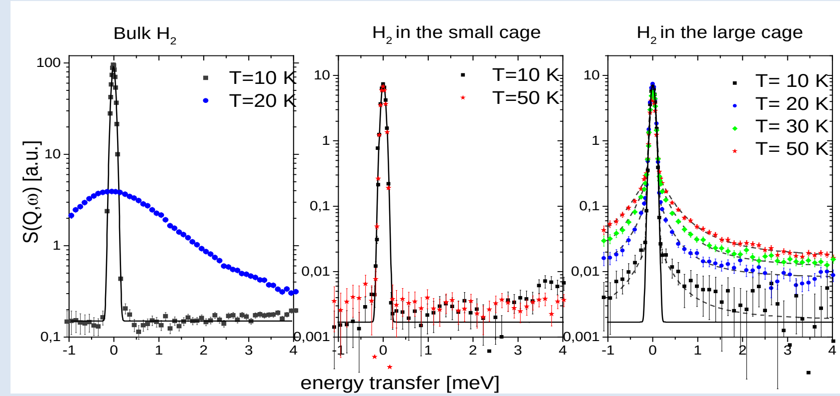
Cation dynamics in hybrid perovskites





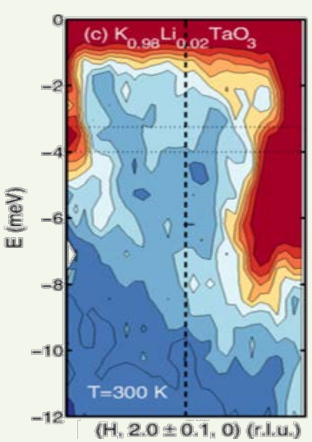
I. P. Swainson *et al*, Rapid Comm. PRB, 2015

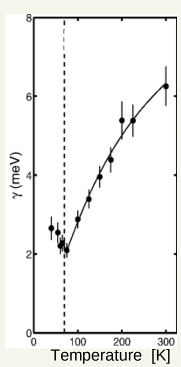
Tuning confined dynamics by the pore size

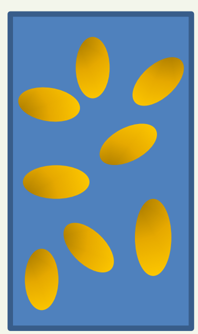


M. Russina *et al*, Scientific Reports, 2016

Fluctuating dipoles in relaxor ferroelectrics

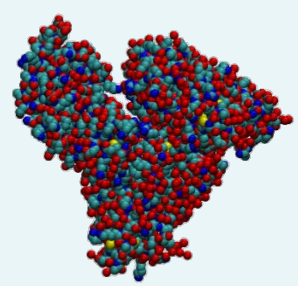


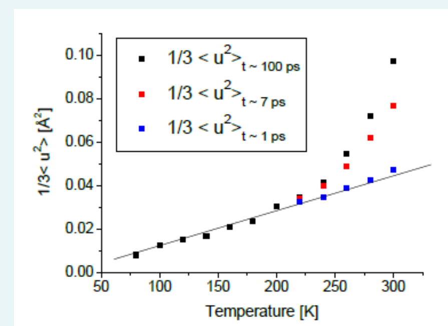




C. Stock *et al*, PRB 90, 2014

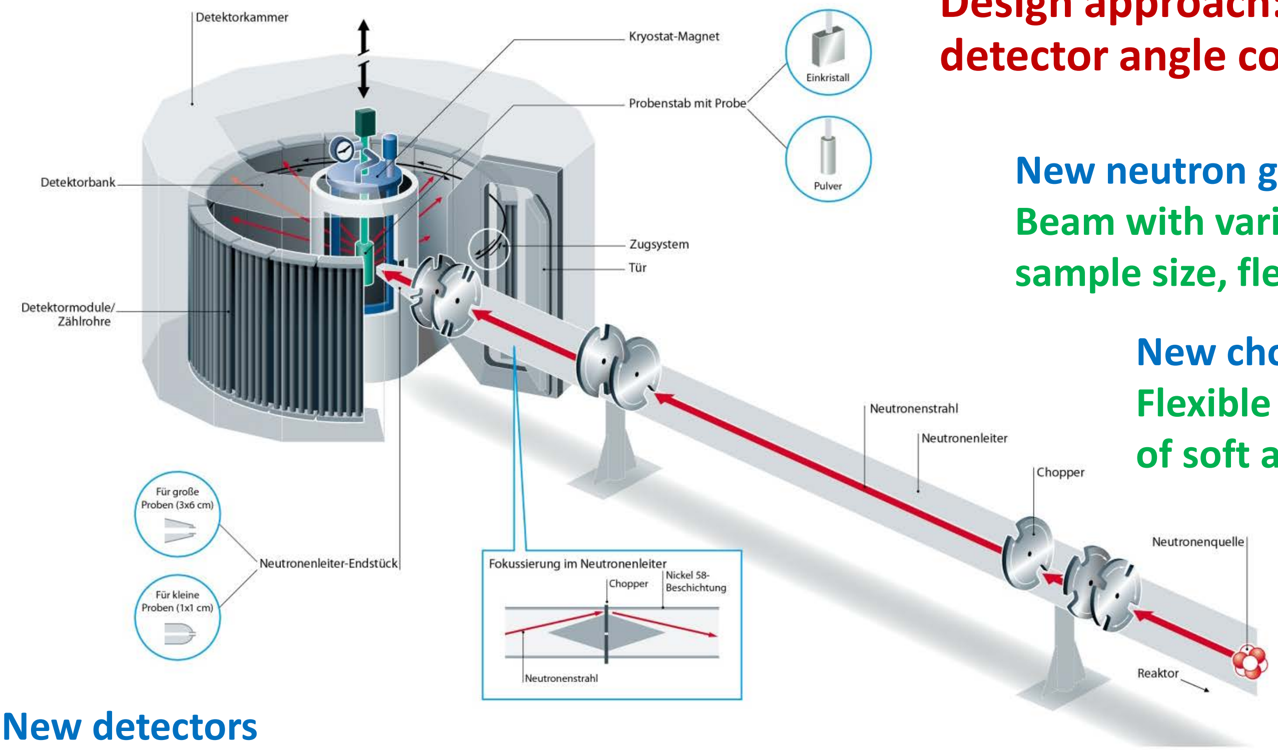
Nature of “dynamic transition” in proteins





S. Magazù *et al*, BBA, 2016

UPGRADE OF NEAT: ADVANCED DESIGN CONCEPT



Design approach: High intensity x Increased detector angle coverage x Flexibility

New neutron guides with various focusing :
Beam with variable properties: flexible sample size, flexible divergence

New chopper system with variable pulses:
Flexible resolution, optimized for studies of soft and hard matter

New detectors
Higher position resolution (3° -> 0.6°)
Higher detector angle coverage

New instrument capabilities:
High magnetic field, single crystals, smaller amount of samples, magnetic filed up to 14 T, in-situ gas pressure 0.1 mbar -200 bar

Upgrade completed in 2016

Broad range of applications: soft matter, magnetism, energy

Access to new science fields: Time-resolved studies, single crystals, high magnetic field

NEAT 2016: TIME LINE

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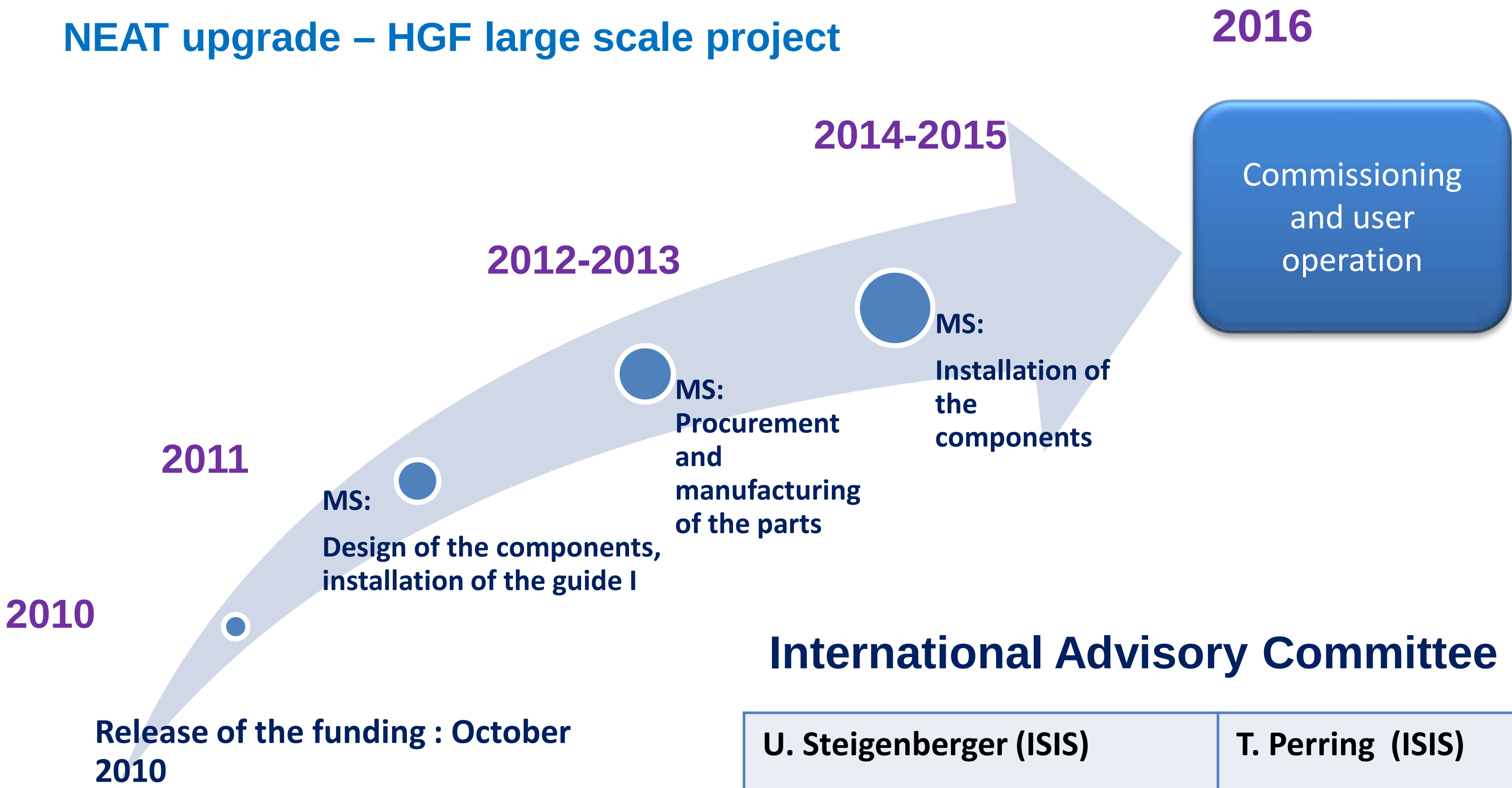
NEAT upgrade – HGF large scale project



International Advisory Committee

U. Steigenberger (ISIS)	T. Perring (ISIS)
H. Mutka (ILL)	B. Guerard (ILL)
M-L. Saboungi (IMPMC)	N. Malikova (LLB)
B. Lake (HZB)	O. Stöckert (MPI Dresden)

INTEGRATED GUIDE CHOPPER SYSTEM

Various scientific application have different sometime contradicting requirements

Filtering of requirements

Science based design

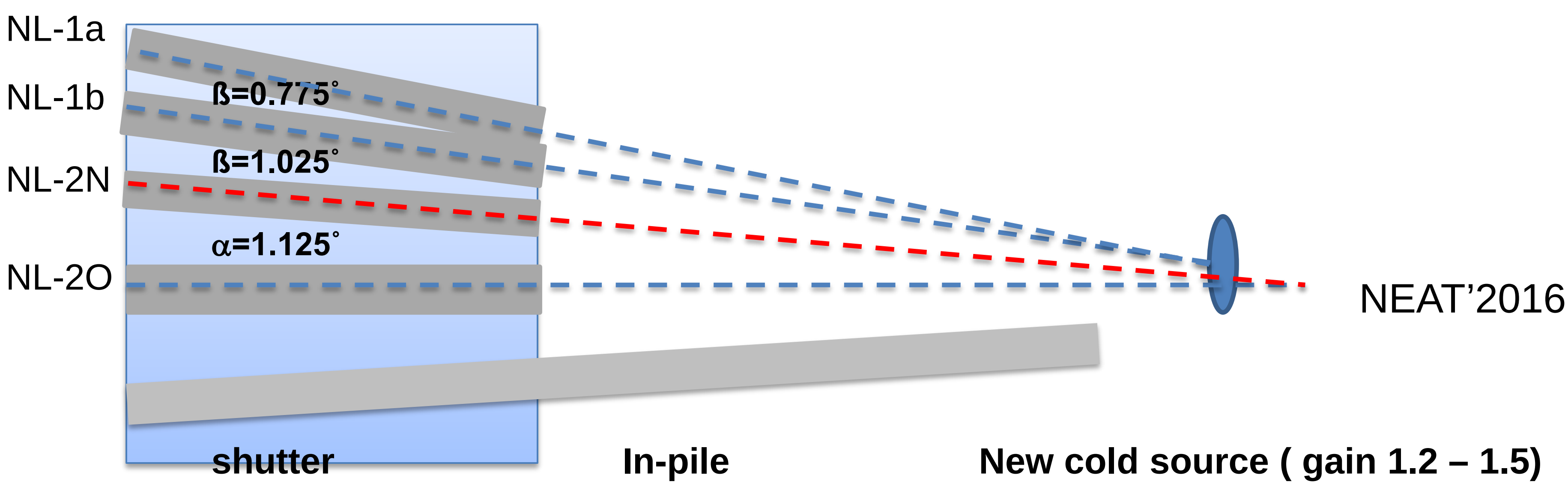
Intensity as a top priority

Matching of guide and choppers geometrical parameters

Minimizing of losses

Flexibility trough exchangeable guide section and various chopper slits

NEAT guide at NL-2N: 125 x 60 mm, m=3Θ_c



Upgrade of the HZB in-pile guide system (T. Krist, A. Tennant, Neutron News 2014/2)

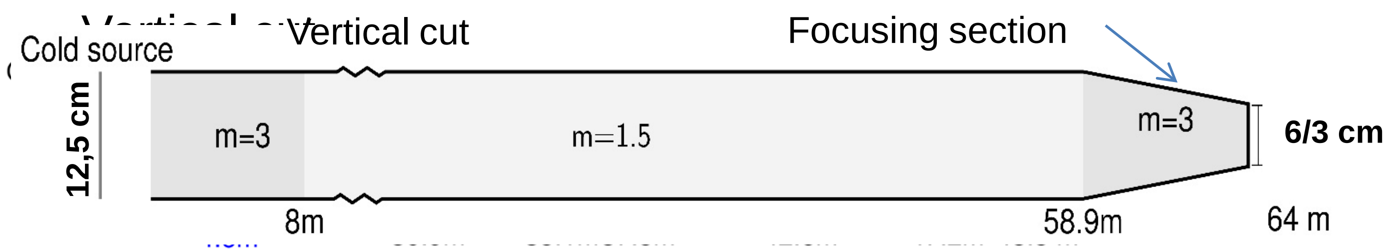
1. **Remove in-pile guide system, replace with SM box, add additional neutron guide**

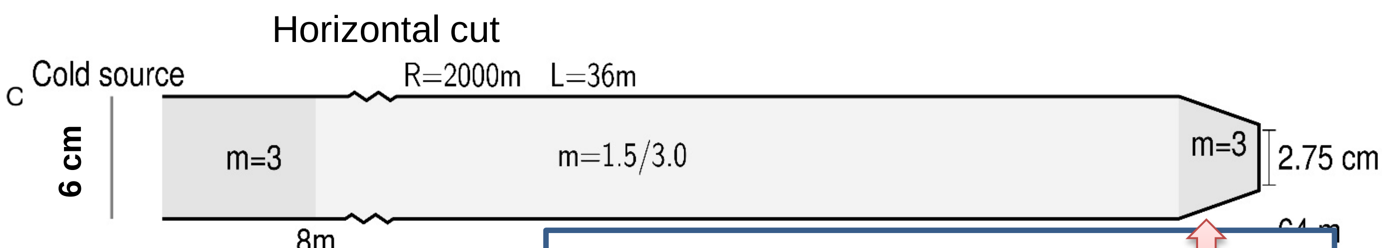
   (F. Mezei, internal HMI report, January 2007)

2. **Change the direction of the guides, increase the dimensions**

   (M. Russina, internal HZB report, April 2008; fine tuning by K. Habicht and T. Krist, internal report June 2008)

NEAT 2016 / NEAT 1995:

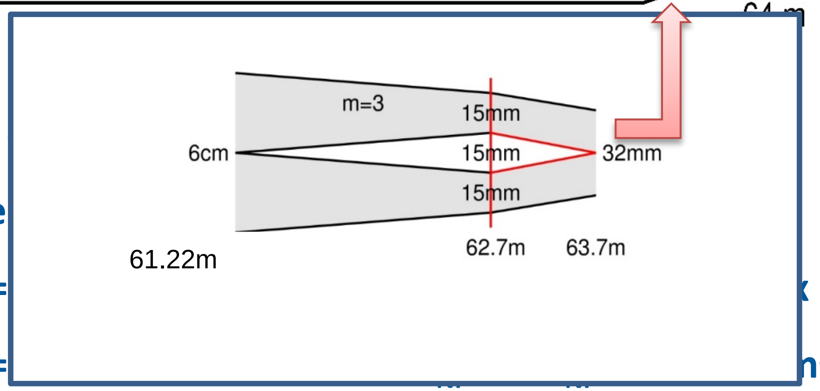




Horizontal cut

- **Neutron guide of larger**

(f = phase space



f_{1995} = … x Θ_{Ni}^2

f_{2016} = … ^{2} x Θ_{Ni}^2

$f_{IN5} = 200\ mm \times 30\ mm \times 1\Theta_{Ni} \times 1\Theta_{Ni} = 6000\ mm^2 \times \Theta_{Ni}^2$

Gain factor **$f_{2016}/f_{1995} = 7$**

STEP II: ADD FLEXIBILITY

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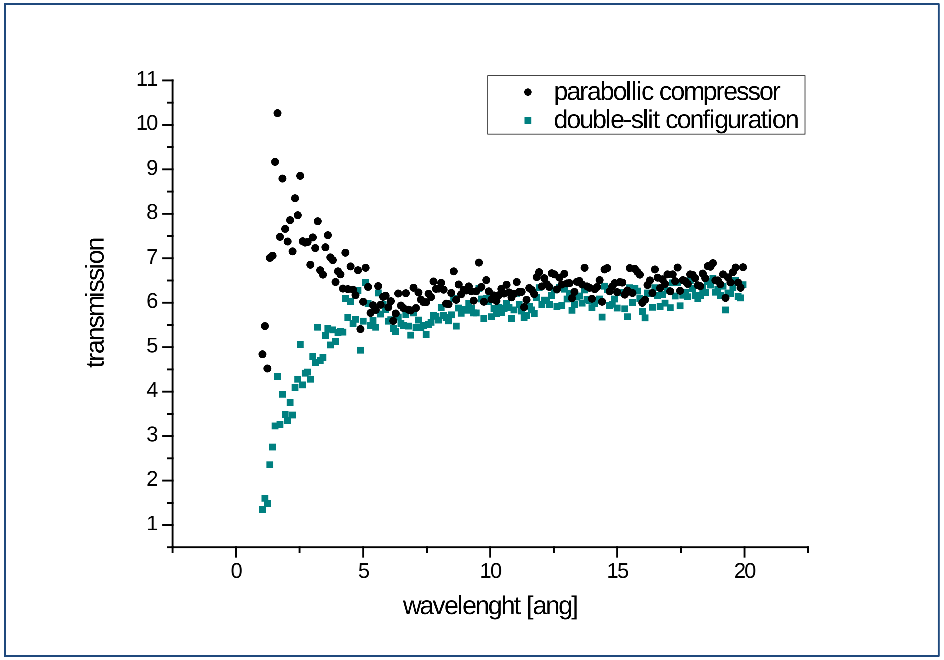
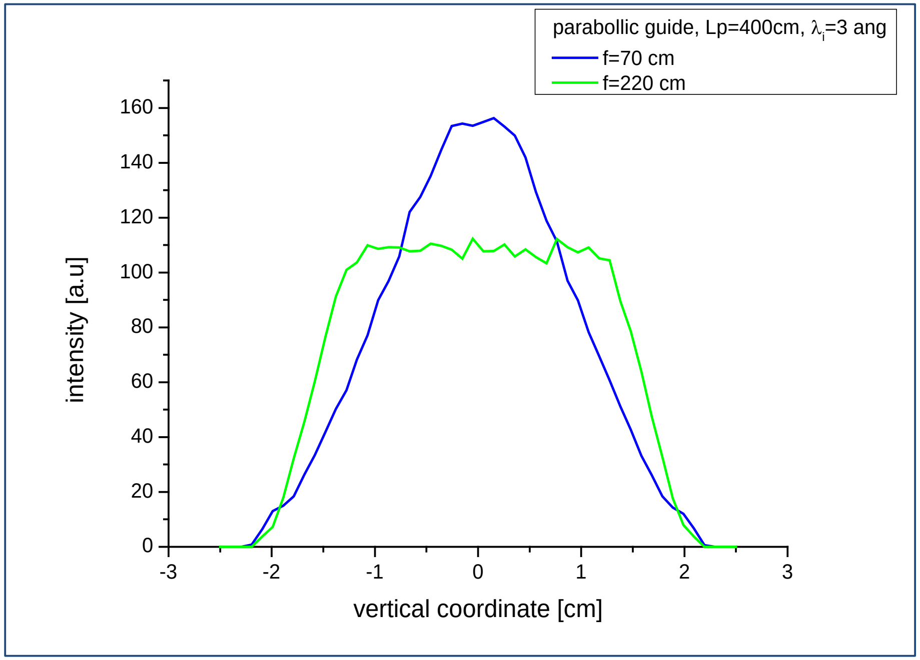
Expected gain factor is confirmed by MC simulations

Various focusing in vertical dimension





Guide #1: parabolic focusing for 3 x 6 samples, homogeneous beam distribution, low divergence

Single crystals, studies with short wavelengths

Guide #2: parabolic "hot-spot" focusing in vertical dimension, double slit compression horizontally for the samples 2 x 3cm

Small samples, high resolution studies, cold neutrons

HIGHLY EFFICIENT AND FLEXIBLE BEAM DELIVERY SYSTEM

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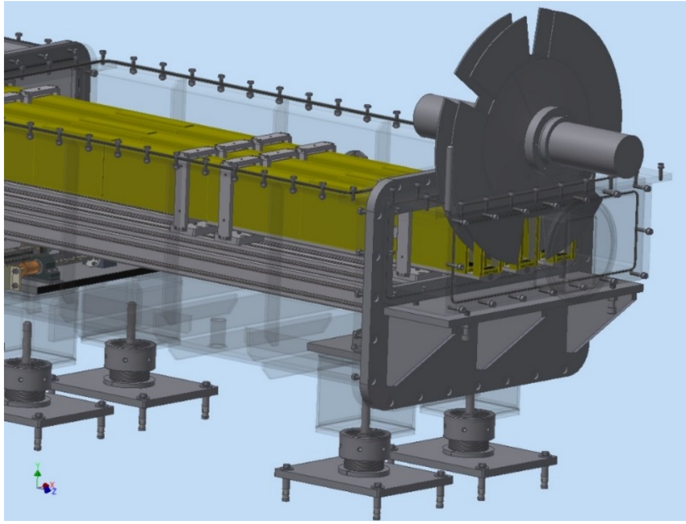
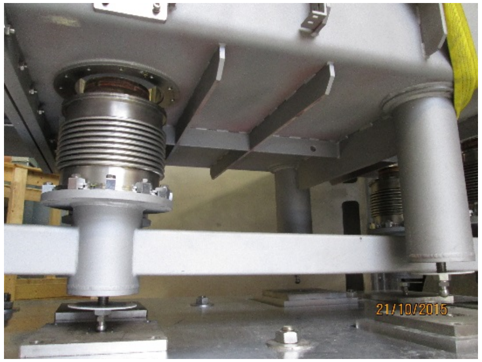
- 70 m of neutron guide has been manufactured and installed by Mirrotron Ltd
- Minimization of losses due joint vacuum for guide and choppers
- Mechanical exchange of two focusing sections
- Continuous quality control during fabrication and installation

Integrated guide chopper design



Two sections for exchange outside and inside detector chamber



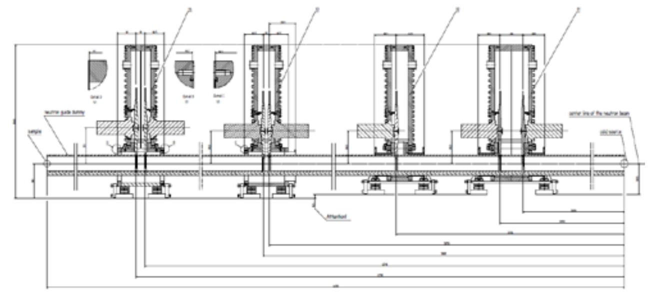
Decoupling of the guide support from chamber

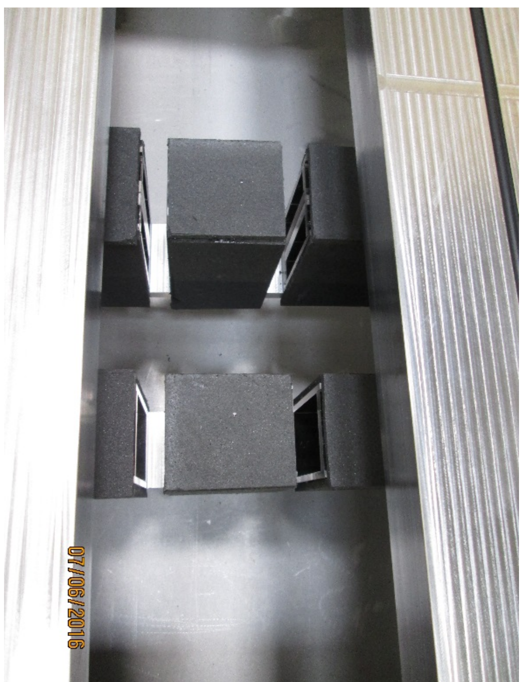
Exchange of the last section in the detector chamber

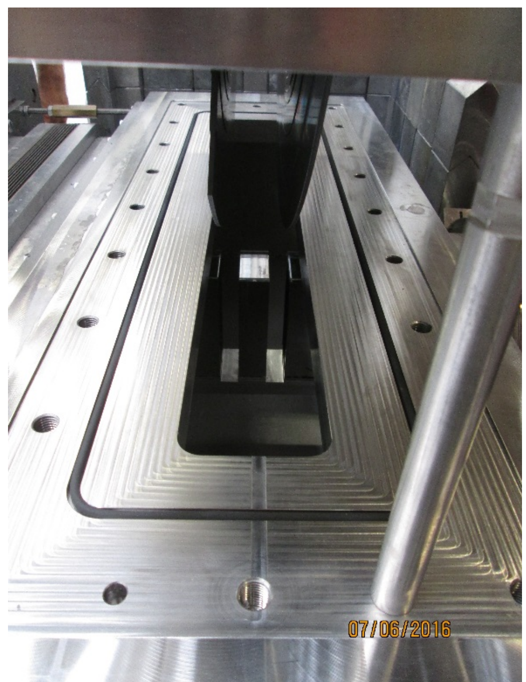
NEAT CHOPPER SYSTEM

- Increase of the length for the primary spectrometer from 12 m to 30 m
- Chopper system from 7 discs produced by ZAT Jülich
- Carbon fiber discs with B_4C coating, passive magnetic bearings
- 300 Hz specified, 110 currently delivered

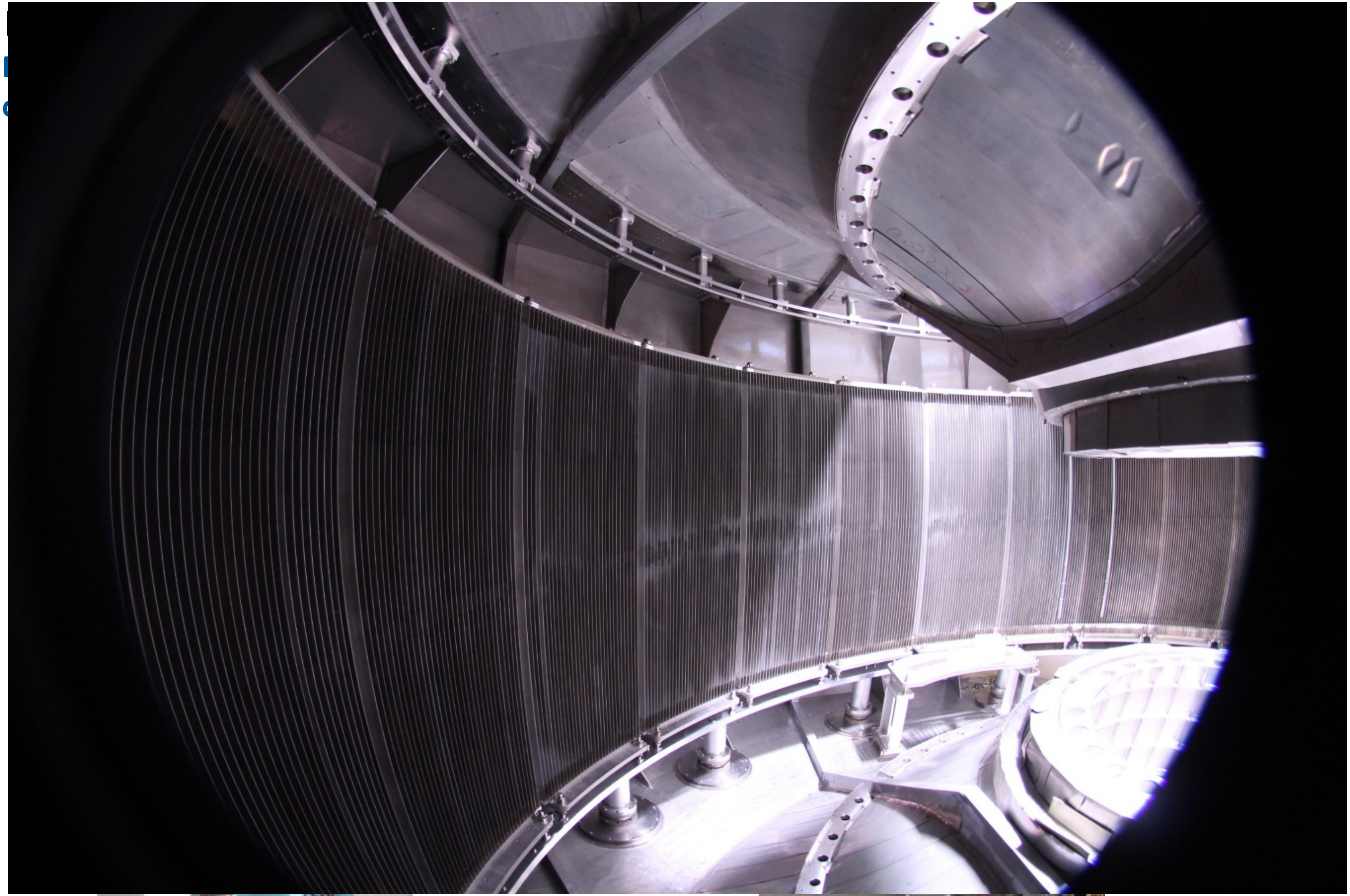
Neat – Chopperkaskade

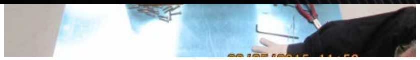


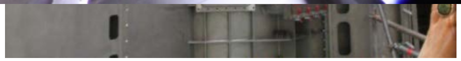




416 3He- detectors, ready to use detector modules and electronics are produced







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Optimization using analytical calculations and VITESS

Transmission: $$t = \frac{V_c}{V_{nc}}$$

Figure of merit: $$G = \frac{SNR_c}{SNR_{nc}}$$

Detection limit: $$C_{DL} \propto \left(\frac{I^2_{sample}}{I_{noise}}\right)^{-1/2}$$

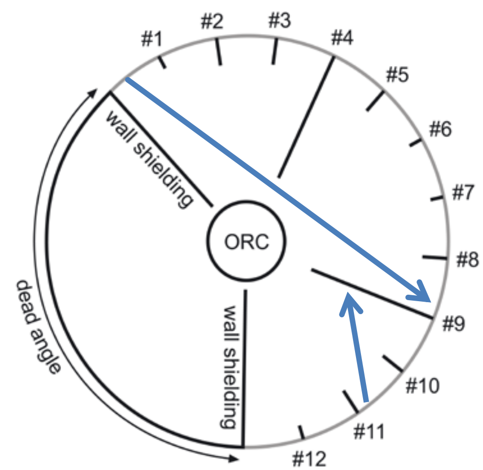
Optimized radial collimator for all sample environment incl. 15 T magnet:

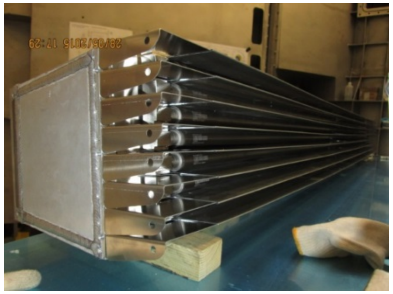
- r_1= 411mm, r_2 = 578mm, 2α = 1.6°
- t ≈ 0.85, G ≈ 10.0

Detector shielding

(a) - 12 module shields

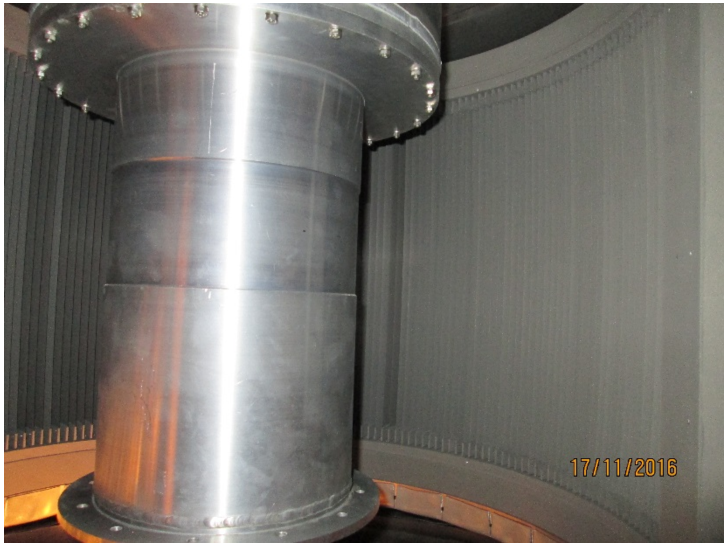
(b) - 415 detector shields (6 cm), offer better performance

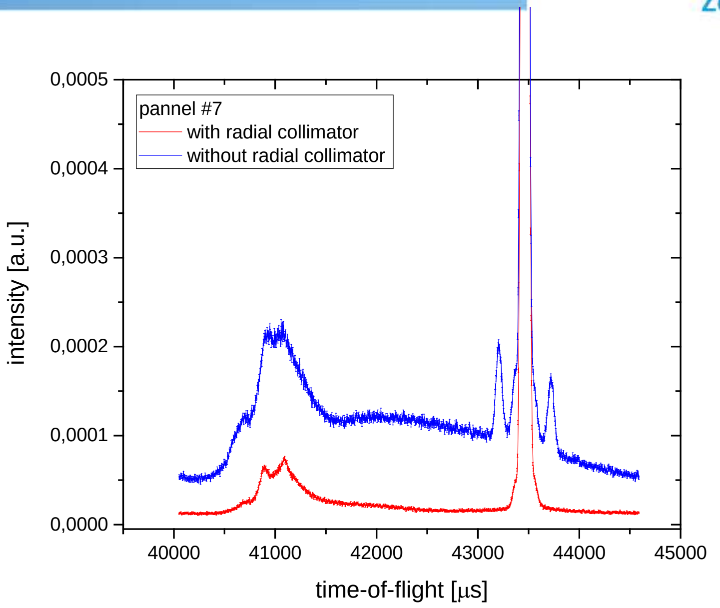




G. Günther, M. Russina in *"Background optimization for the neutron time-of-flight spectrometer NEAT"*, NIMA 828 (2016) 250–261

MINIMIZATION OF THE BACKGROUND





- Collimator produced by JJ X-Ray A/S Denmark
- Further measures include implementation of shielding of Cadmium and borated polyethylene

NEAT 2016: ON THE WAY TO USER OPERATION

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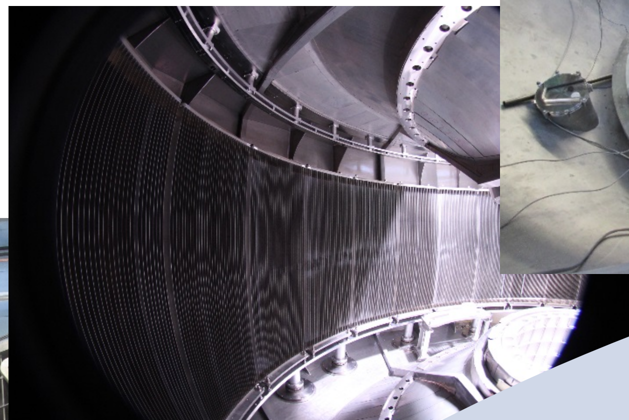
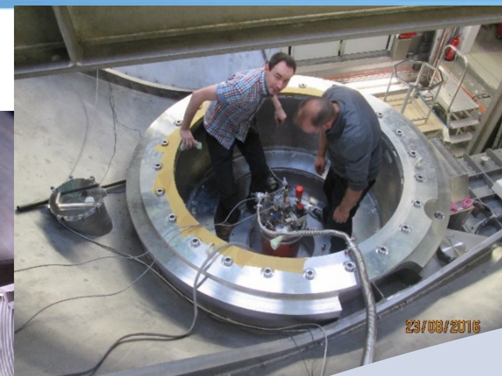




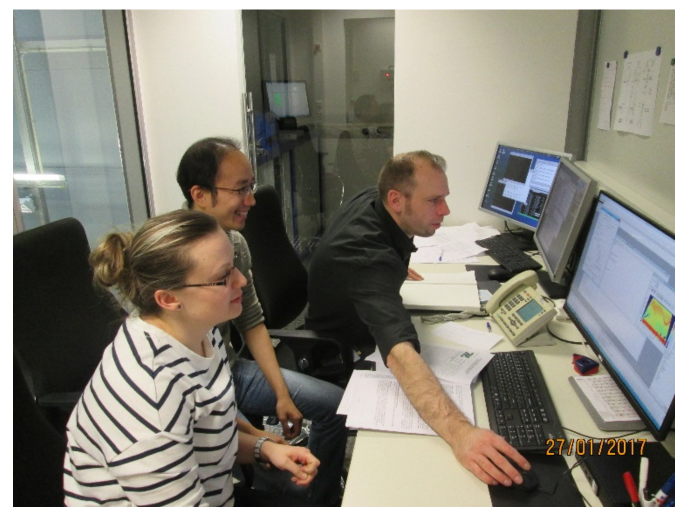
June 2016: installation of choppers and detectors is completed

June 2016: Start of commissioning, first spectra

August 2016: first experiment

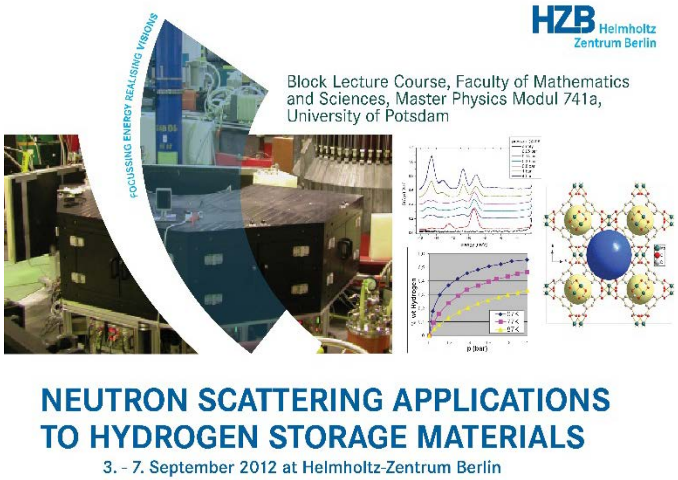
September 2016: first user call, high number of proposal received

January 20, 2017: First regular users



Successful user operation from the start, overbooking factor 2

Annually since 2012: H_2 storage summer school



International conference QENS / WINS 2016

University of Dresden
Prof. Kaskel, Simon Krause

University of Bath / UK
Mi Tian

University of Tartu/ Estonia, Heisi Kurig and Prof. Enn Lust, Carbon 2016

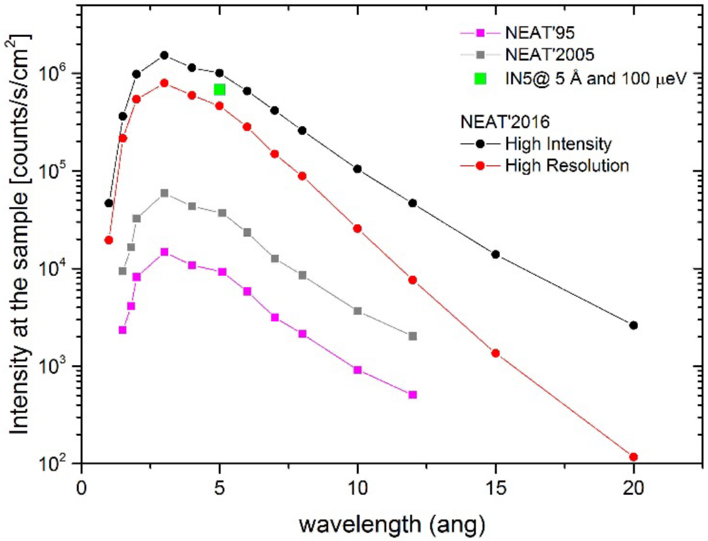
Kurchatov Institute Moscow, Roman Svetogorov, PCCP 2016

University of Kiel/Germany
Helge Reinsch and Prof. N. Stock
PCCP 2016

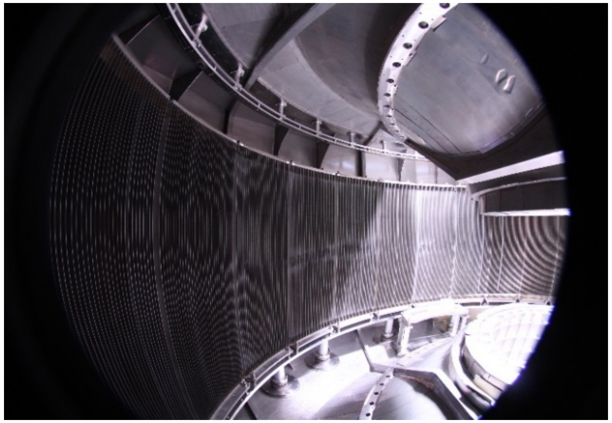
NEAT 2016: PERFORMANCE ON THE LEVEL OF THE WORLD BEST

HZB Helmholtz Zentrum Berlin

Intensity on the sample: x 50 NEAT'1995



Increased detector angle coverage: 6 x NEAT'1995



Low background

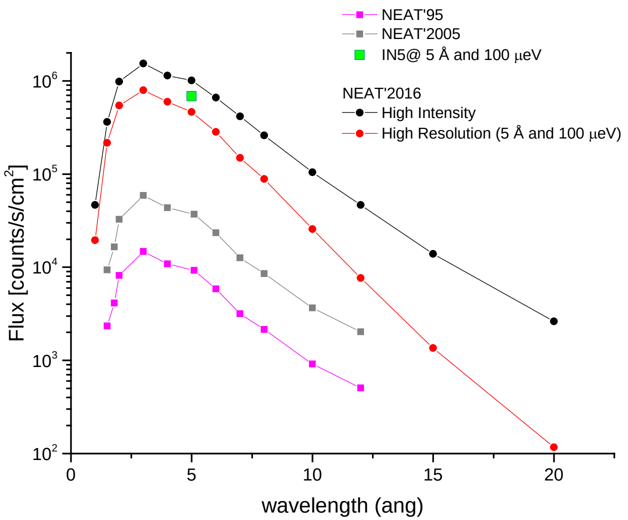
- **High count rate: NEAT'2016 = 300 x NEAT'1995 , <u>similar performance as world leader IN5 at ILL</u> despite of an order of magnitude difference in cold neutron flux**
- **Bispectral spectrometer: 1.3-20 Å @NEAT'2016 vs 2-12 Å @NEAT'1995**
- **Low background: signal to noise ration of ~ 10^4**
- **High instrumental flexibility not compromising the instrument performance**

G. Günther et al, NIMA A 828 (2016) 250–261

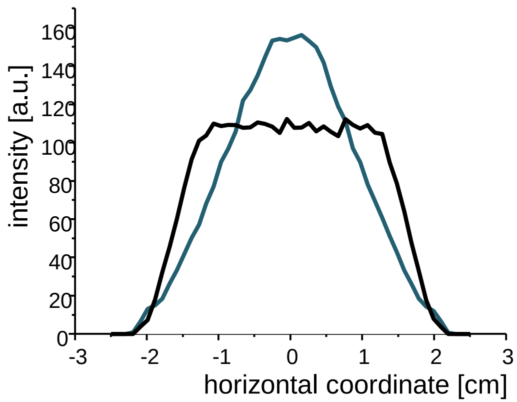
M. Russina et al, Physica B 2017, doi:10.1016/j.physb.2017.12.026

Instrumental capabilities

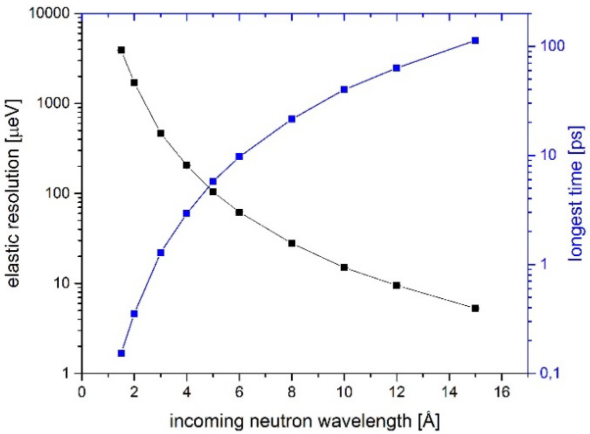
High intensity on the sample



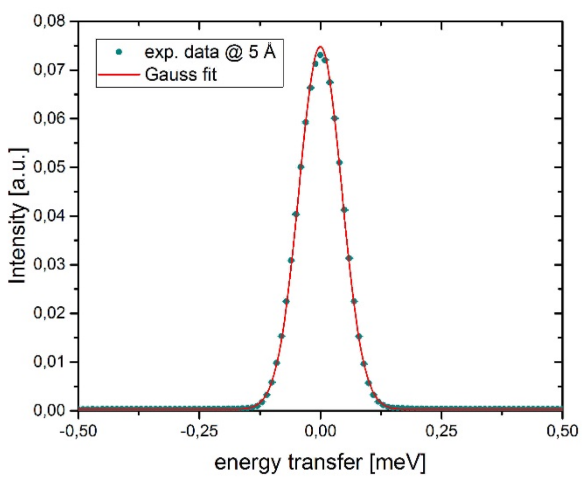
Beam focusing



Dynamics up to 100 ps at Current chopper speed



Nice resolution shape



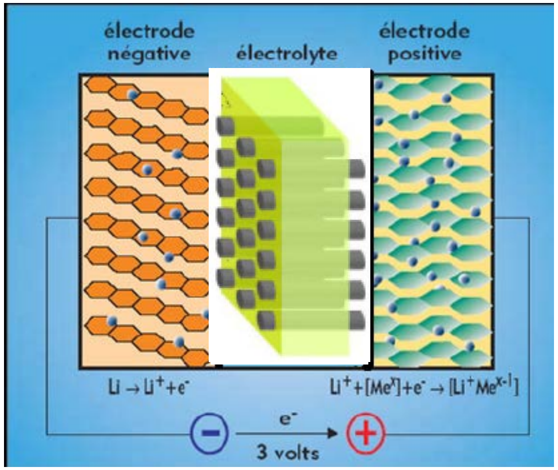
Elastic line width (FWHM) at 5 Å = 102 μeV
Flux = 4.72 x 10 ^{5} n/ s / cm^{2}

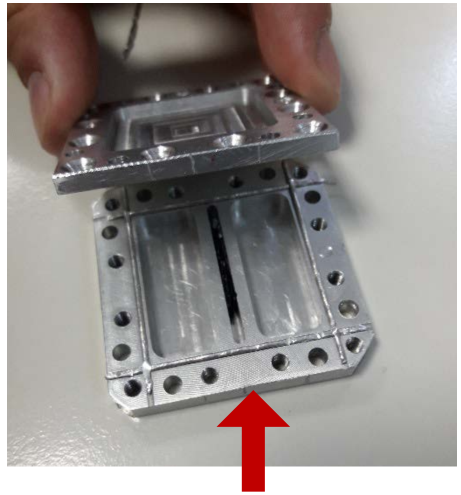
TOFTOF:
Elastic line width (FWHM) at 5 Å = 104 μeV
Flux 1.14 x 10 ^{5} n/ s / cm ^{2}

NIMA 580 (2007) 1414–1422

J.M. ZANOTTI, Q. BERROD, P. JUDENSTEIN (CEA SACLAY AND CNRS, FRANCE

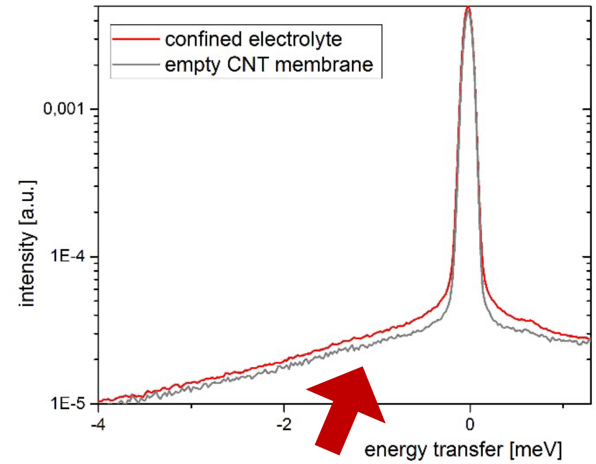
HZB Helmholtz Zentrum Berlin





5 mg of confined electrolyte
70 mg of CNT membrane

NEAT'2016



~~Confined ionic diffusion~~

Not possible at NEAT'2005

1D Confinment:

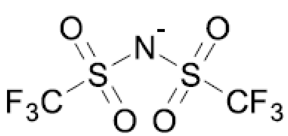
Frustration of IL self-organization

Pore size (1-3 nm) ≤ nano-organization (~2 nm)

Specific arrangement of molecules, no friction

ANIONS

TFSI

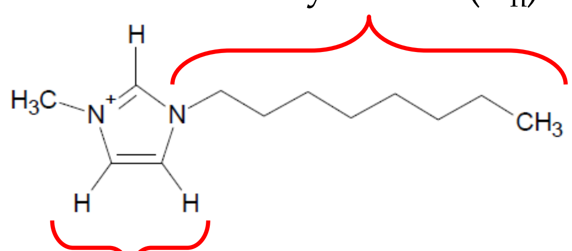


trifluoromethylsulfonyl-imide

Br^- Cl^- BF_4^-

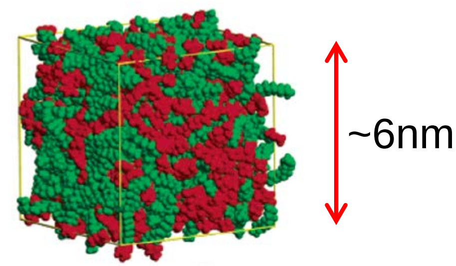
CATIONS

Alkyl chain (C_n)



methyl-imidazolium (MIM)

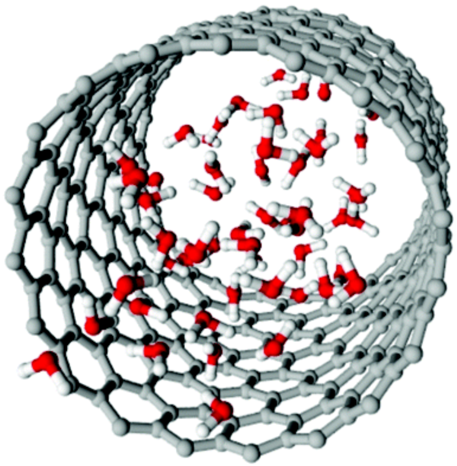
Self-organization



Padua et al. *J. Phys. Chem. B*, **2006**

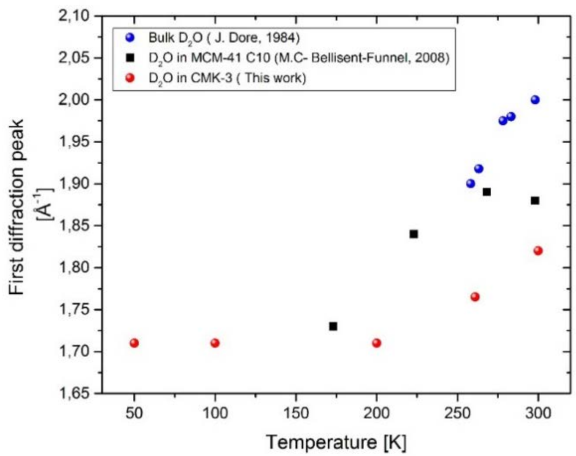
Instrumental capabilities

- Transport in human body and living organisms
- Catalysis
- Energy applications / batteries, energy storage, fuel cells and etc.)
- Geology and Environment
- Building construction (clays, cement …)
- And many others



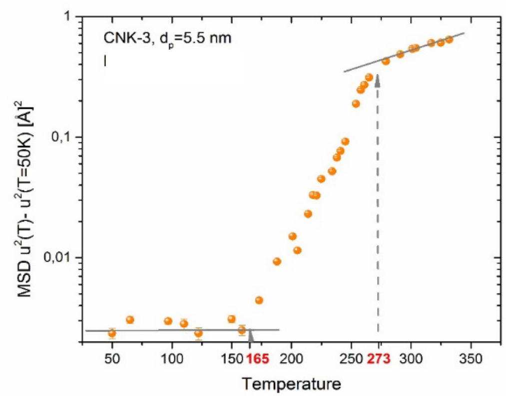
5-20 mg of D_2O in 90 mg of porous material

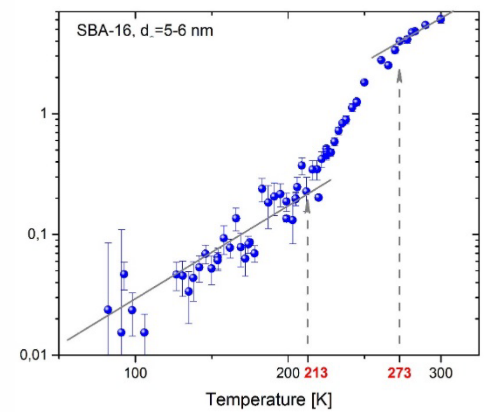
Structure of confined water



Mobility of confined water

MSD in hydrophobic and in hydrophilic environment





M.C. Schlegel (BAM, HZB), V. Grzimek (HZB), A. Petrova (University S. Petersburg) *et al.*

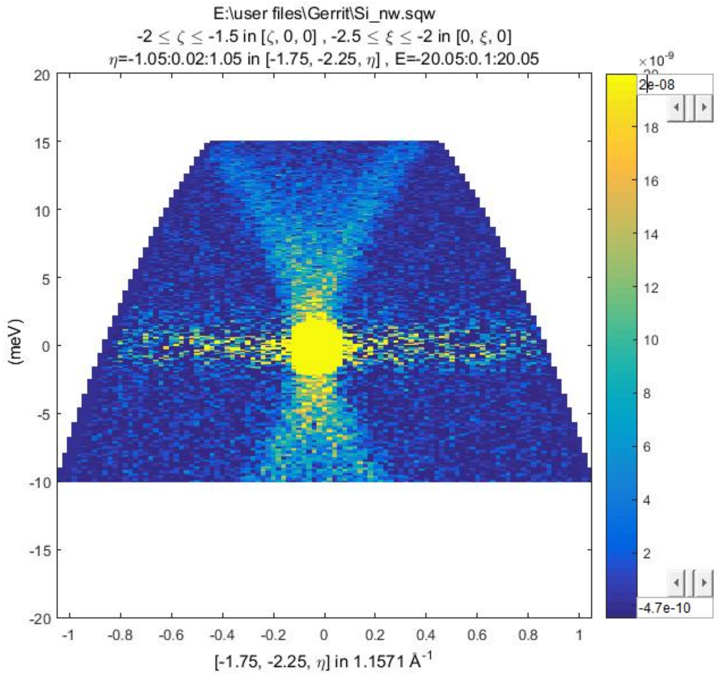
DPG 2018, CPP 79.2 Mar 16 2018, 9:45-10:00, PC 203

Better position resolution

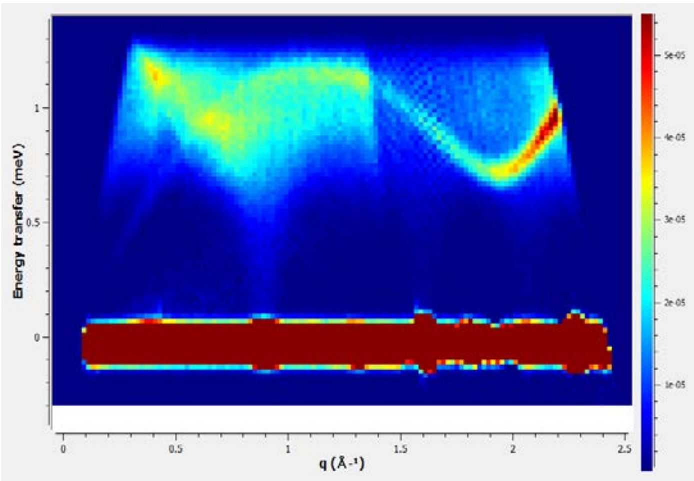
HZB Helmholtz Zentrum Berlin

416 position sensitive detectors:

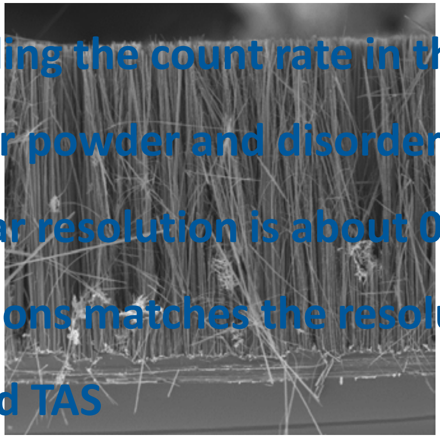
- **Filled with 3 bar ^{3}He**
- **11-18 mm vertical position resolution**
- **25 mm horizontal position resolution (ca. 40 000 pixels)**
- **1 π solid angle coverage**
- **Event recording**



Following steep dispersion



Single crystal studies



- Doubling the count rate in the range of 2Θ ≤ 90° for powder and disordered samples

- Angular resolution is about 0.5° in both dimensions matches the resolution of standard TAS

BETTER CONDITIONS FOR IN-SITU STUDIES

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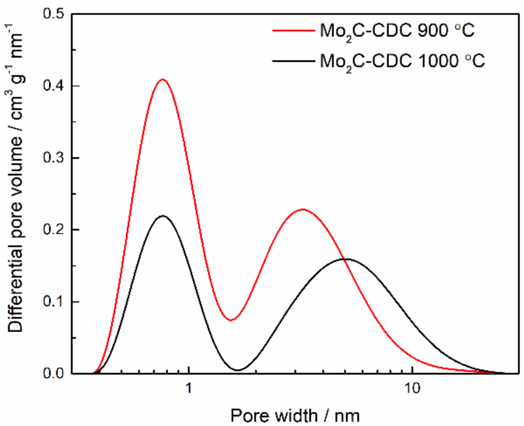
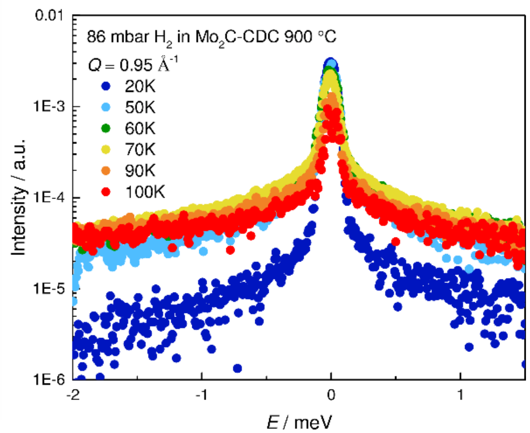
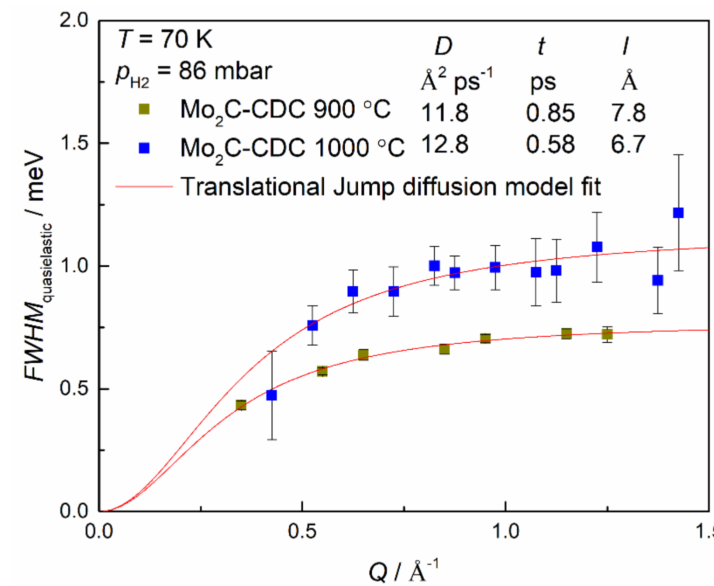
Sample environment for in-situ gas controlled experiments in wide range of pressures of 10 mbar -200 bar

Example: mass transfer in metal derived porous carbon.



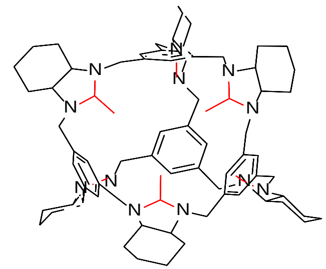


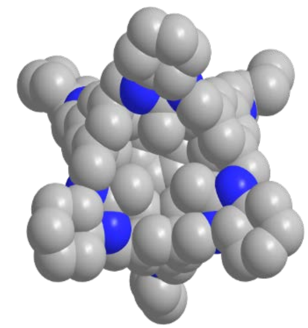
Measured diffusion coefficient



Heisi Kurig, Rasmus Palm, Uni Tartu/ Estonia

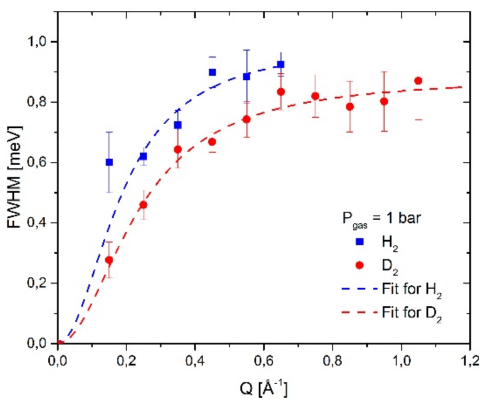
Sample environment for in-situ gas controlled experiments in wide range of pressures of 10 mbar -200 bar

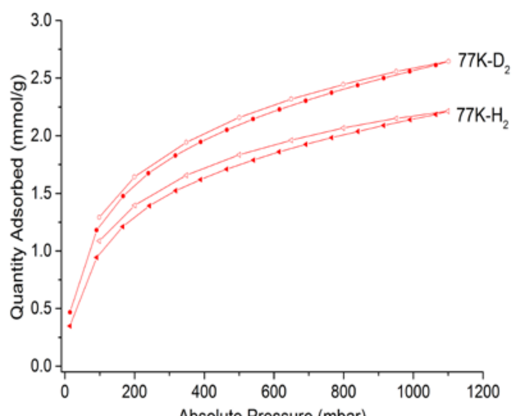




Example: hydrogen isotope separation at elevated temperatures

T=77K





T= 77 K

D_s (H_2) = 21,37±4,64 [Å^2/p]

D_s (D_2) = 12,0689±1,101 [Å^2/p]

Mi Tian (University of Bath) and the group of Prof. A. Cooper (University of Liverpool)

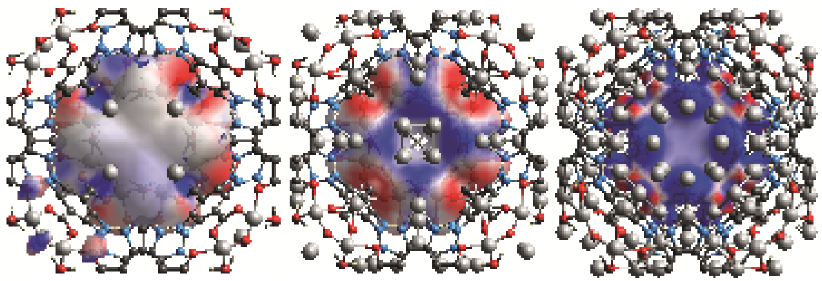
Better conditions for low temperature studies

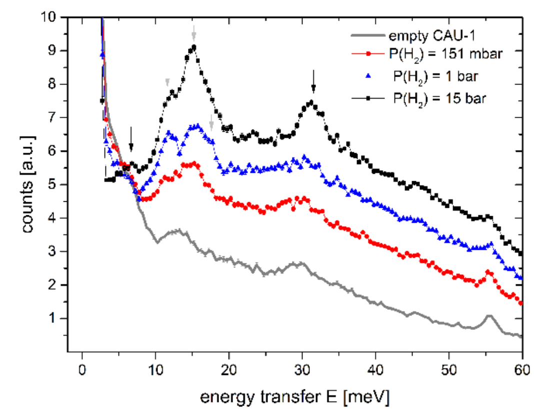
HZB Helmholtz Zentrum Berlin

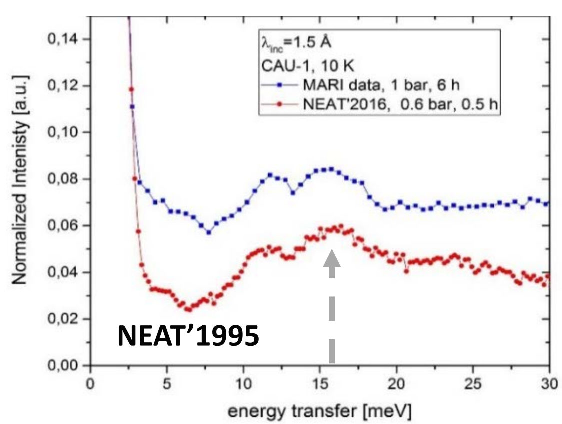
- **High intensity allows access to broader wavelength range:** **1.3-20 Å @NEAT'2016 vs 2-12 Å @NEAT'1995 >= Doubling of frequency range at energy loss => better conditions for low temperature studies**

Example : hydrogen storage in metal organic framework CAU-1

Adsorption induced contraction of CAU-1 structure leads to rearrangement of H_2 molecules and the formation of new positions







Structural changes lead to changes of quantum rotational states

M. Schlegel, M. Russina et al, Phys. Chem. Chem. Phys. 18 (2016) 29258, DOI: 10.1039/C6CP05310F

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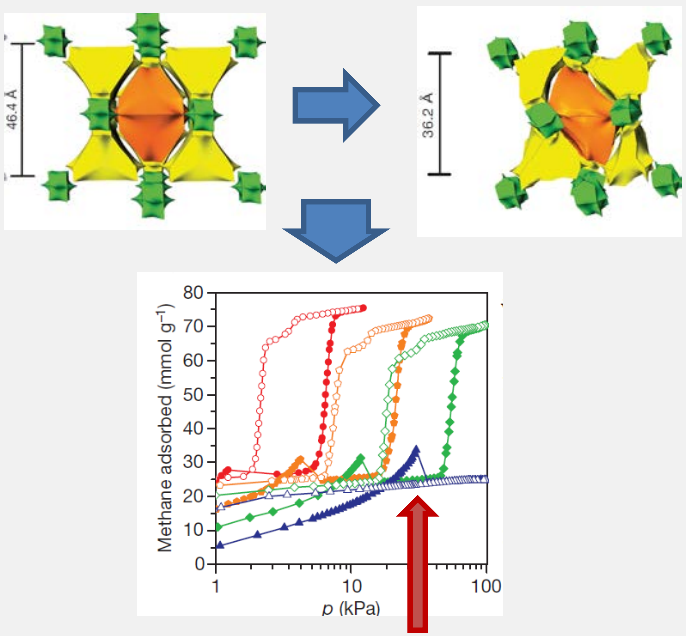
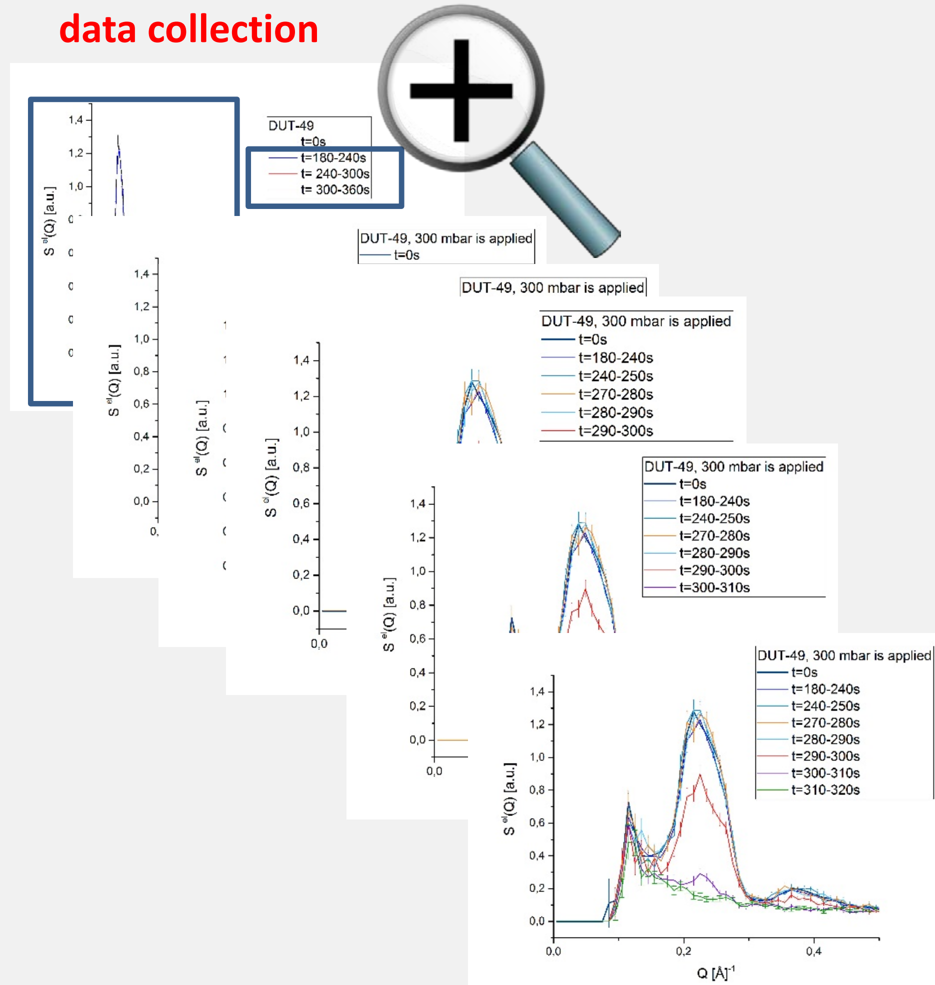
Gas confinement in MOFs:

Expelling of the gas due to the deformation of the structure upon gas loading and onset of guest-host interactions

NEAT'2016: Following structural changes in real time within 1 s time resolution

Key: in-situ gas pressure + event recording data collection





LETTER

doi:10.1038/nature17430

A pressure-amplifying framework material with negative gas adsorption transitions

Simon Krause[1*], Volodymyr Bon[1*], Irena Senkovska[1], Ulrich Stoeck[1†], Dirk Wallacher[2], Daniel M. Többens[3], Stefan Zander[3], Renjith S. Pillai[4], Guillaume Maurin[4], François-Xavier Coudert[5] & Stefan Kaskel[1]

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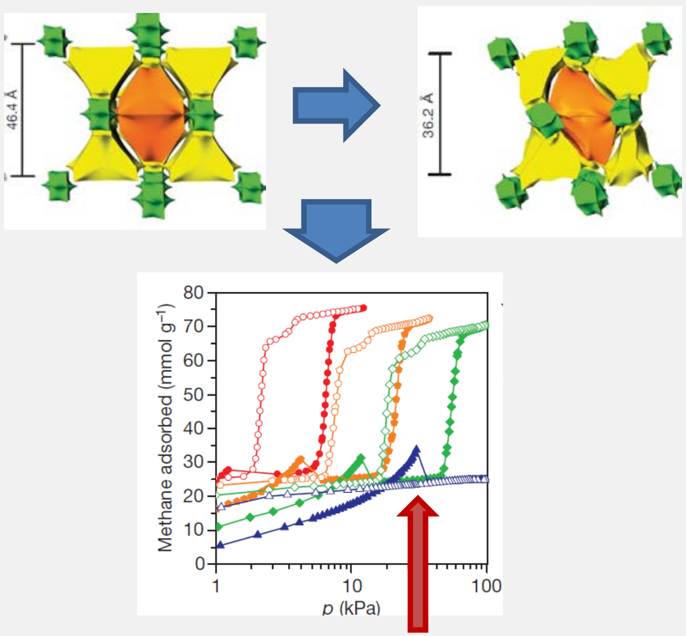

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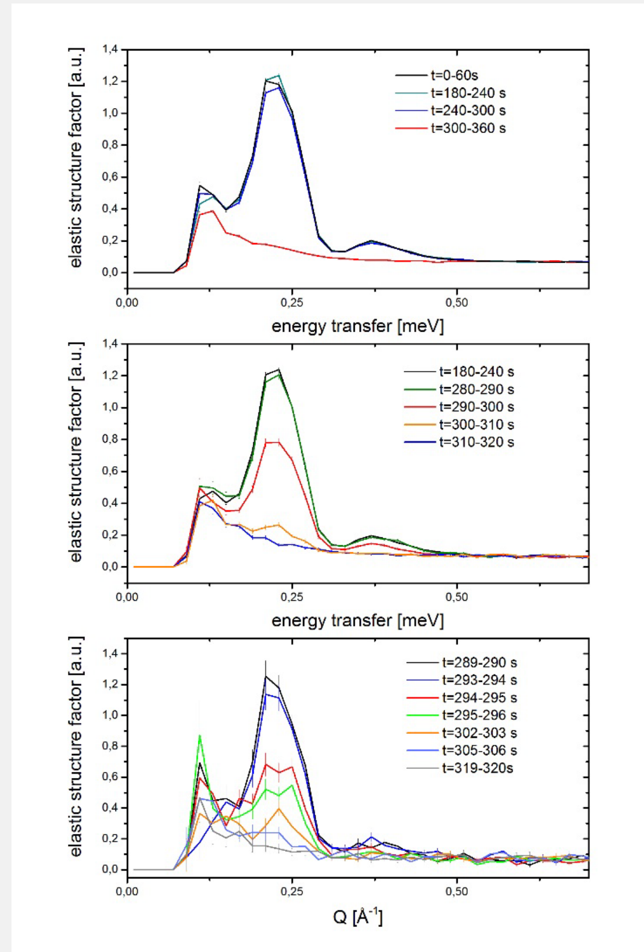

ADVANCED SAMPLE ENVIRONMENT

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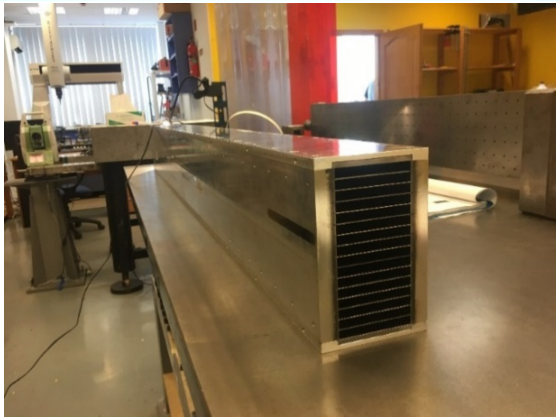
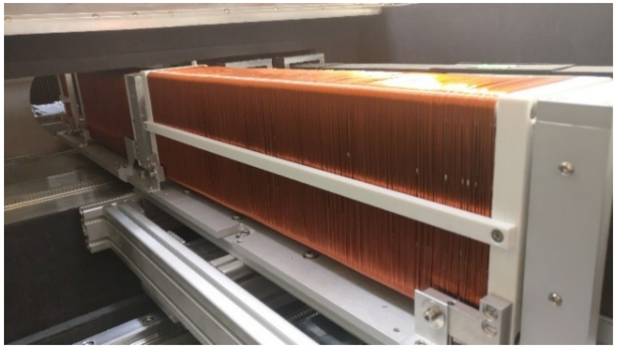
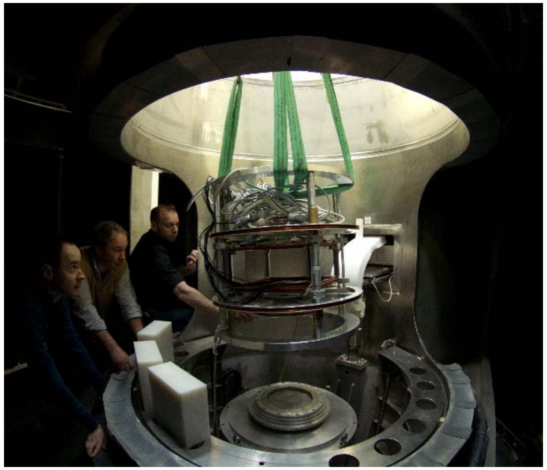


Temperature range 40 mK – 1000 K

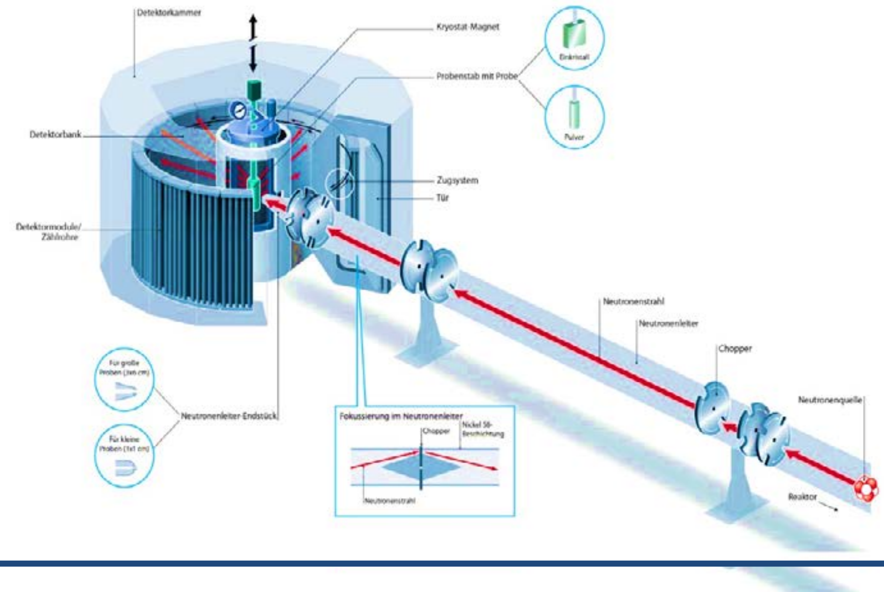
High field magnet up to 14 T

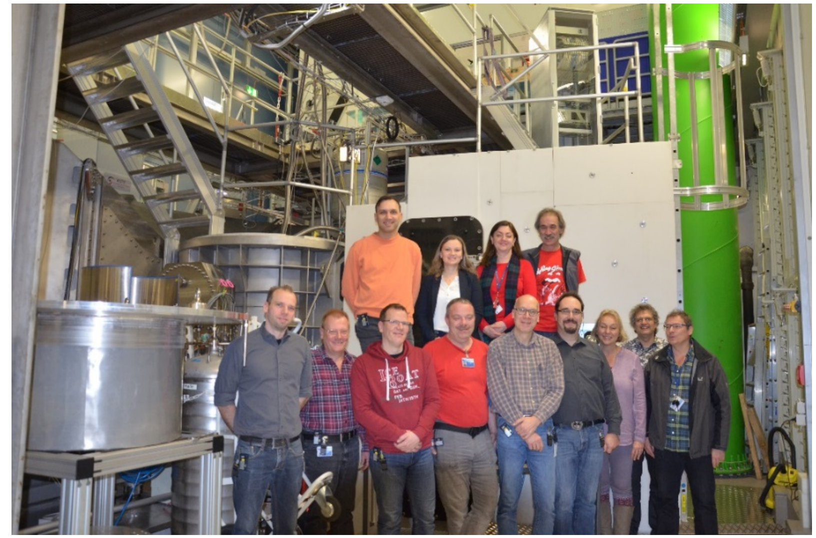
Polarized neutrons in broad wavelength range





NEAT 2016





- **NEAT'16 is a powerful, state-of –the art neutron "nanoscope" to study dynamics at nanoscale**
- **NEAT'16 ~ 300 x NEAT'95 , similar performance as a world leader IN5 in France**
- **High intensity, instrumental flexibility and new capabilities enable high data rate, complex experiments, novel studies**
- **Broad range of applications, user operation started, contact:**

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