Software requirements for MIRACLES - The backscattering spectrometer at ESS

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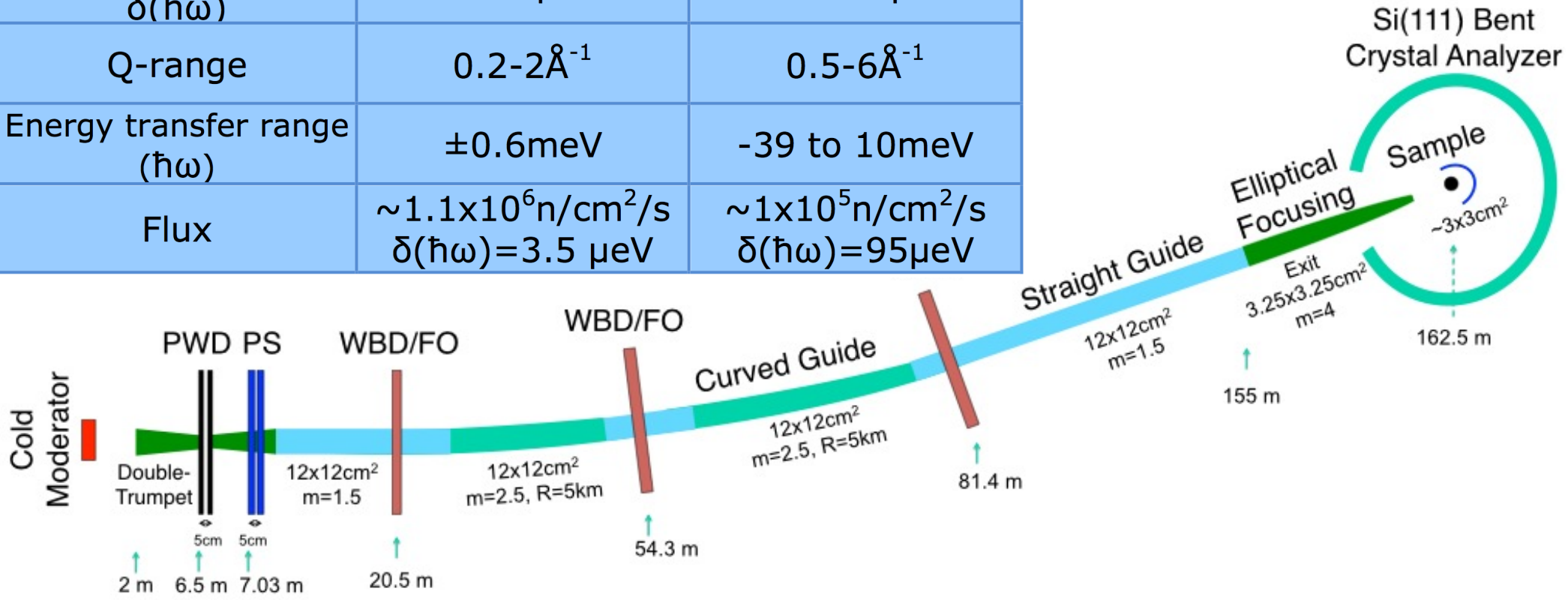
Disentangling time distribution

Analyzer crystals	Si(111) (6.267Å)	Si(333) (2.08Å)
energy resolution - δ(ħω)	2-32 μeV	25-350 μeV
Q-range	0.2-2Å^{-1}	0.5-6Å^{-1}
Energy transfer range (ħω)	±0.6meV	-39 to 10meV
Flux	~1.1x10^{6}n/cm^2/s δ(ħω)=3.5 μeV	~1x10^{5}n/cm^2/s δ(ħω)=95μeV



For δ(ħω)=3.5 μeV the flux at BASIS is 1.4x10^{5}n/cm^2/s

At 5Å (δ(ħω)~95 μeV) the flux at IN5 is 6.3x10^{5}n/cm^2/s and at C-SPEC 1.5x10^{6}n/cm^2/s

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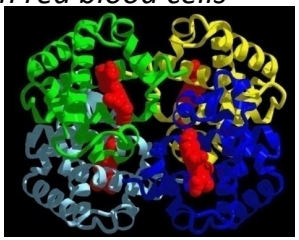
N. Tsapatsaris et al; Rev. Sci. Instrum., ***87****, 085118 (2016)*

Science Case

Life science

Dynamics of Proteins and Water

Example: Self-diffusion of haemoglobine and water diffusion in human red blood cells

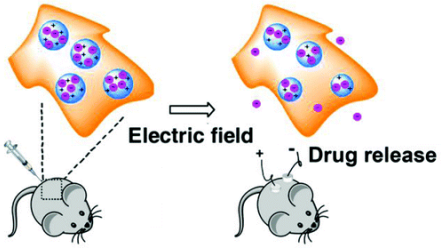


M. Stadler et al., Biophysical J. 95, 5449 (2008)

Pharmaceutical science

Drug Delivery

Example: drug release from electric-field responsive nanoparticles

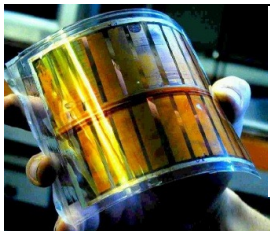


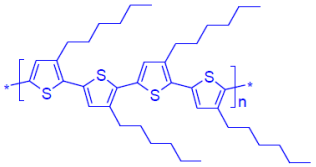
J. Ge et al., ACS Nano. 6, 227-233 (2012).

Polymer science

Morphology-performance connections

Example: Polymers in organic photovoltaic devices



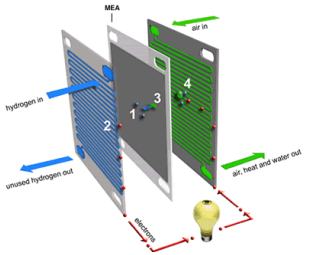


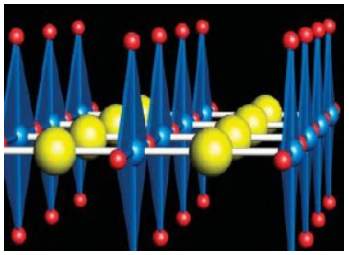
G. Paternó et al.,Chem. Phys.427, 142 (2013)

Energy science

Fuel Cells – Hydrogen Storage

Example: Hydrogen conduction in the solid state



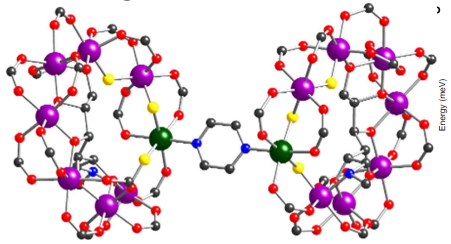


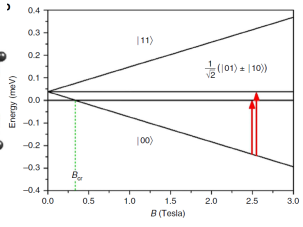
M. A. Haywarth et al., Adv. Mater. 18, 3304 (2006)

21st century Magnetism

Quantum Information Processing

Example: Molecular magnets and quantum entanglement



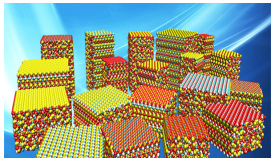


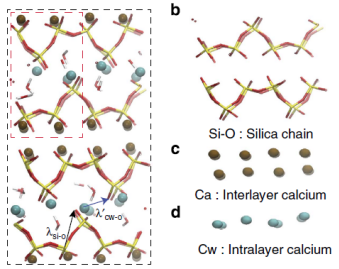
E. Garlatti et al., Nature Commun. 8, 14543 (2017)

Environment science

Greener building materials

Example: use of greener cements to reduce greenhouse gases [a]





J. Jacobsen et al., Sci. Reports 3, 2667 (2013)

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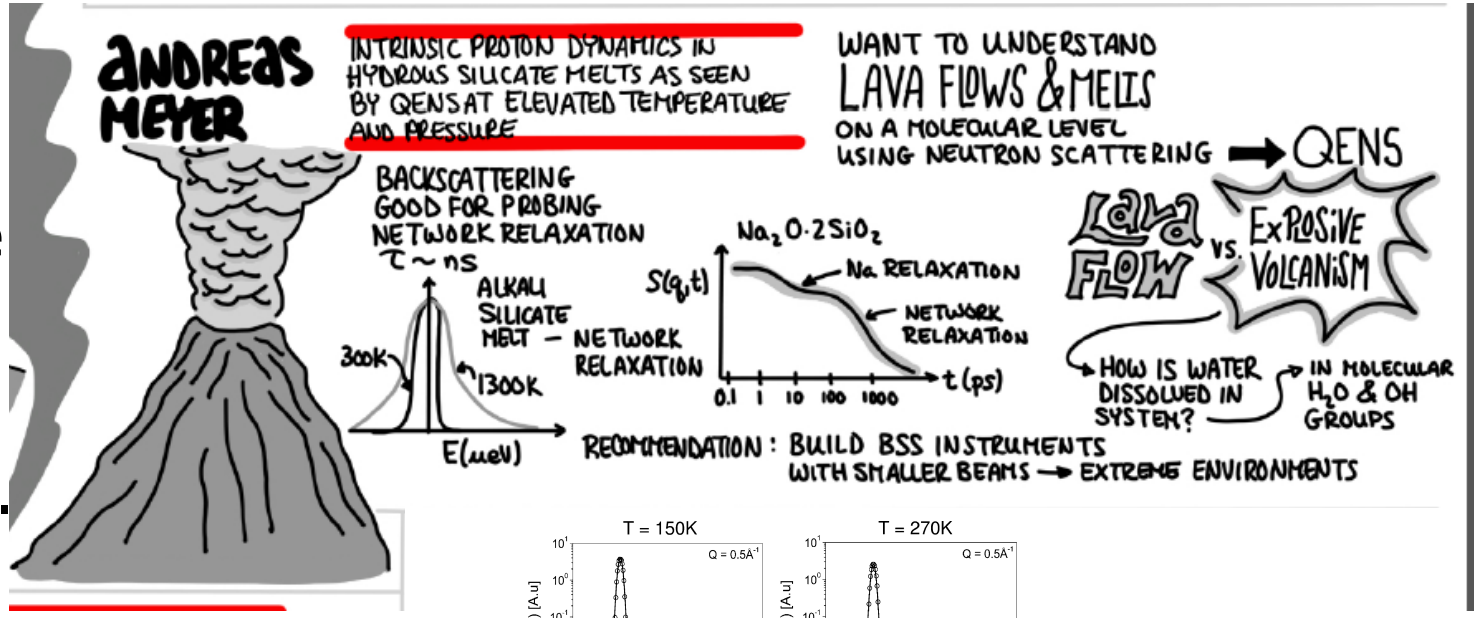
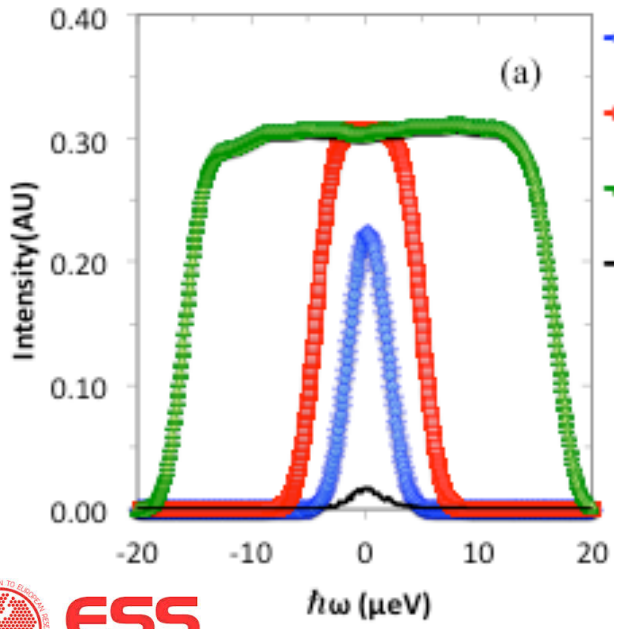
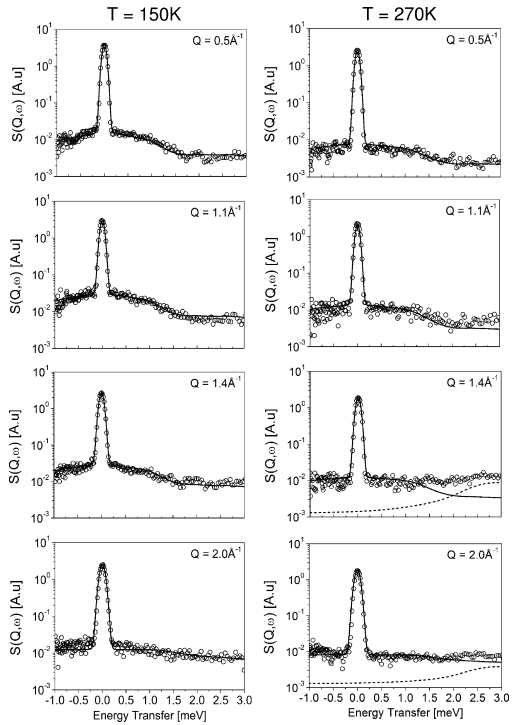
MIRACLES brings a **paradigm shift to neutron backscattering**

- ☑ Outstanding signal/noise ratio.
- ☑ Very large Q-range and even broader elastic energy resolution coverage.







A. Desmet et al, J. Phys. Chem. C, ***115****, 12689 (2011)*

Validation of the MD potential and development of a model reproducing the guest molecule dynamics.

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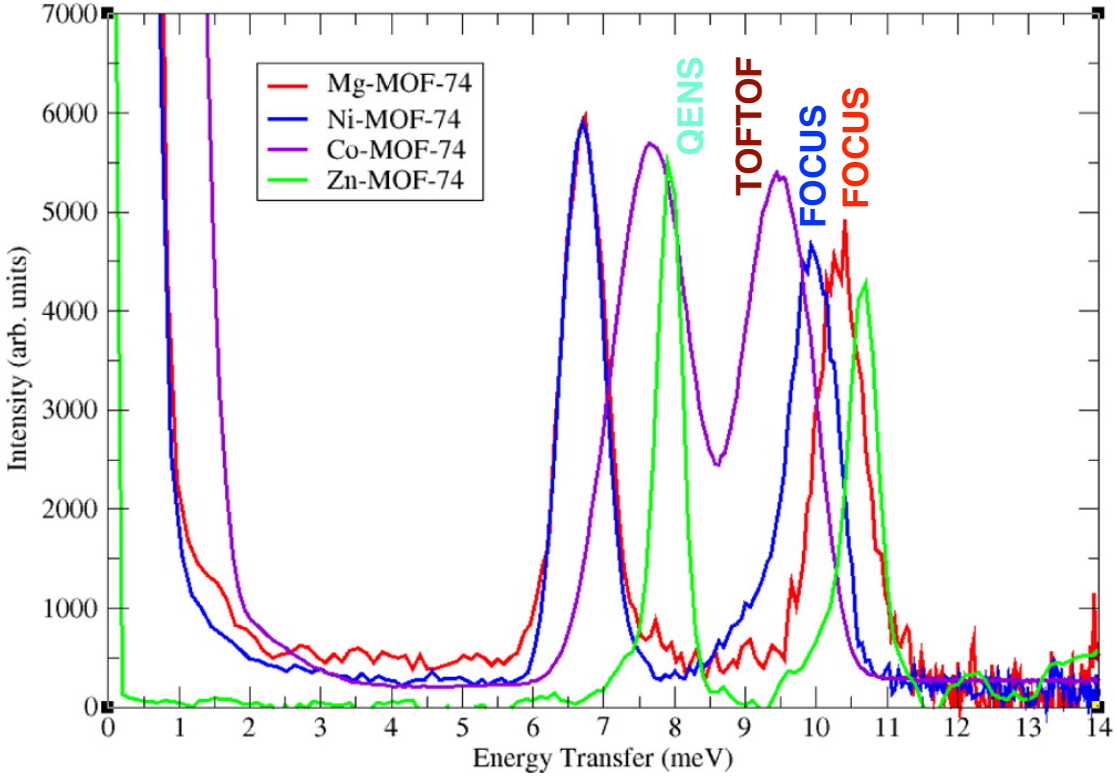
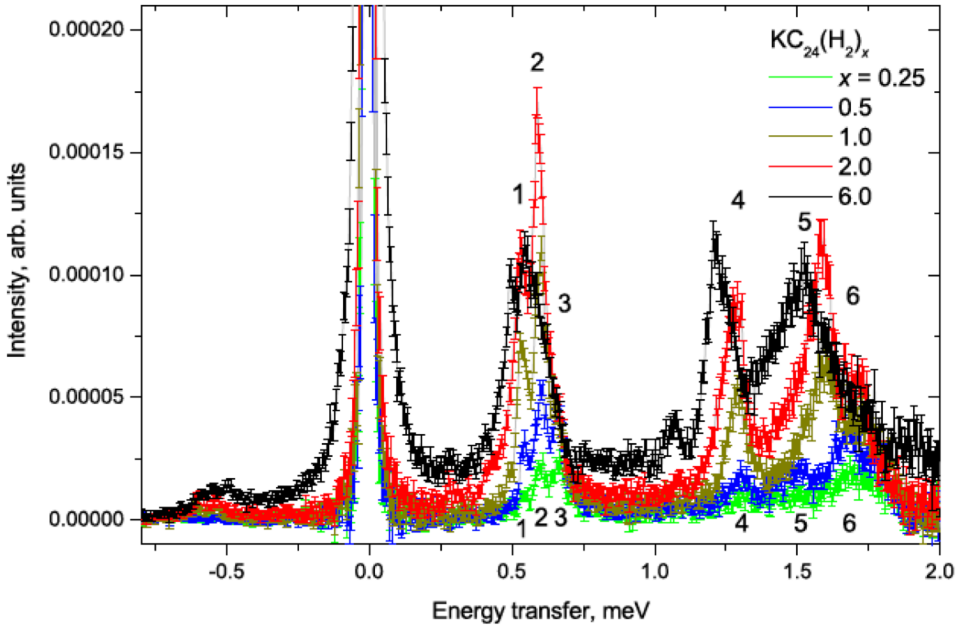
Working on Inelastic Mode

Hydrogen Storage: H2 in porous systems



Pham, T. et al, *J.Phys.Chem. C* **2015**, 119, 1078.

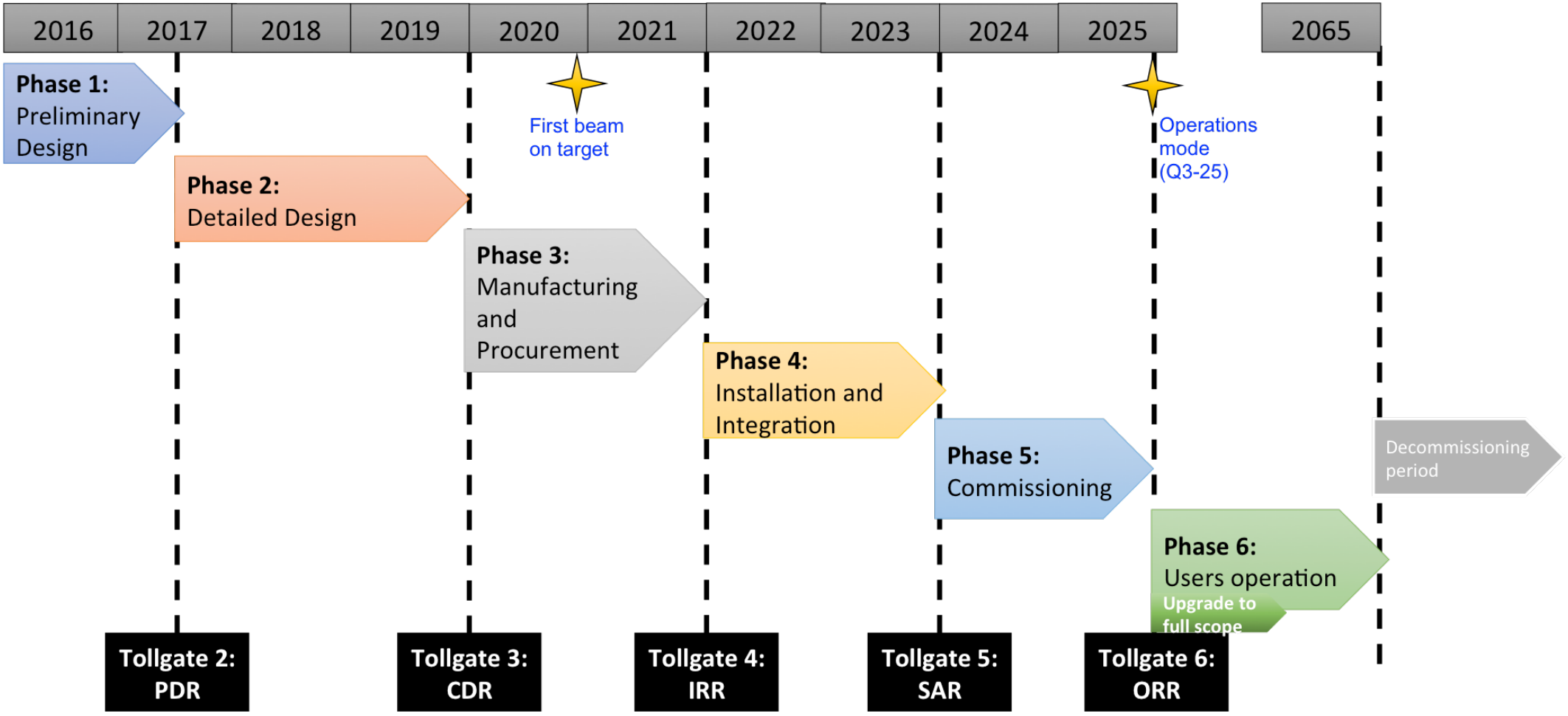
Hydrogen Storage: Molecular hydrogen binding



Lovell, A.et al *Phys. Rev.* Lett **2008** 101, 126101.

FOCUS and TOFTOF collected with 2Å; QENS at IPNS ΔE= 90μeV; IRIS ΔE= 54μeV

MIRACLES project timeline



Script control

Script + GUI control

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Basic reduction

GUI reduction
Automated 'live' reduction

Components to be controlled:

- chopper configurations, wavelength (defined either in chopper terms (expert) or resolution terms (user))
- slit
- shutter
- sample stage / stick
- sample environment (many parameters)
- in situ SE: control SE and run simultaneously
- vacuum, cooling
- (resetting server connections)

- minimise time for changing instrument configuration
- log file - incl. some info on e.g. count rates, SE parameters

- for expert: remote access and control
- for user: web page with main run parameters (when off site)

Minimal requirements that shall be available already prior to commissioning to avoid delays as well as to make on-line data processing easier by allowing quick detection of problems:

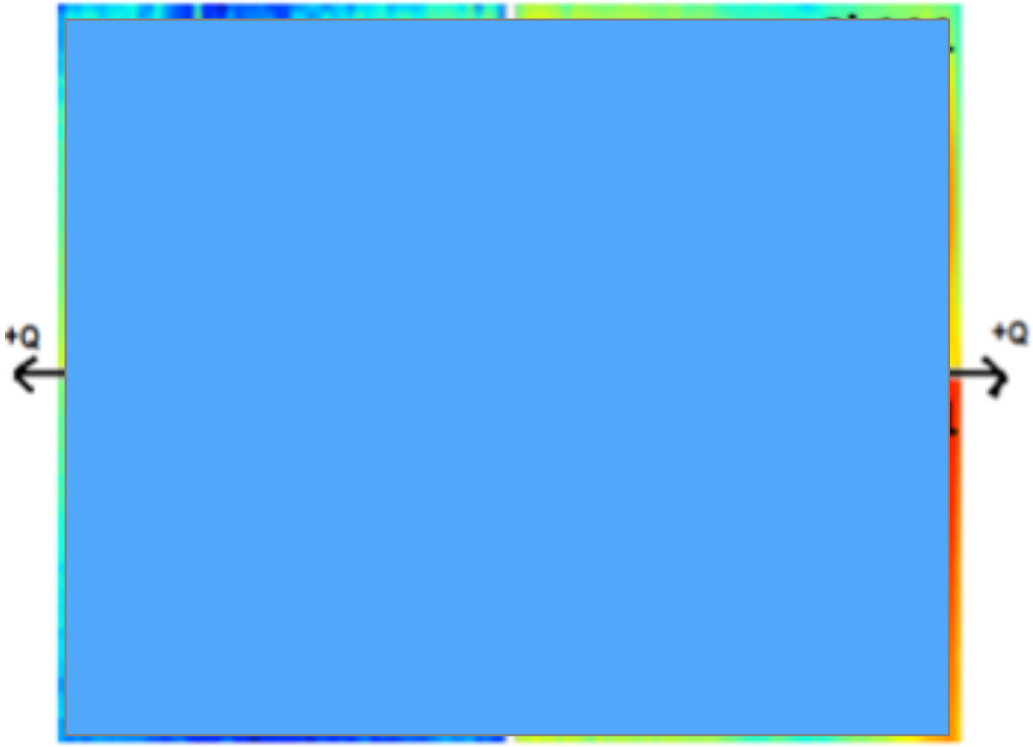
Defining T_0 and $T_{Chopper0}$

ESS timing interface: only collect data when ESS running at 14 Hz

Chopper control system: This part of the software shall provide for scanning the delay time (phase angle) either offline or automatically/ live. The integrated spectra, plotted against phase angle/delay time, can be obtained either by collecting the data at specific monitors or at a range of detectors/ pixels.

Detectors and Analysers: If detectors are non-linear or have false junctions, their electronics will have strong harmonic signals implying software is needed to process for calibration positions that also enable viewing the LPSD tubes. This software must also provide for ToF/energy focusing correction for each pixel due to the correlation between the Bragg angle θ_B and the flight path change. For example, on BASIS the lack of correction increases the elastic resolution from 3.5μeV to 5μeV.

Analyser panels reflection variations: Because the Si(111) panels will be made by pressing the crystals over a large area, there will be reflectivity variations across the panels Therefore a calibration/ correction for vanadium + vanadium / detector tube efficiency need to be performed.



Count intensity for a sample measured on BASIS. The color scale goes from high detected intensity in red to low detected intensity in yellow/green for the Si(111) analyzers. Each square represents a different crystal analyzer panel. The arrows show Q = 0 $Å^{-1}$ in the middle and it increases towards the edges.

Specific run modes: The software should allow for defining the run/scan type. Therefore, one needs to be able to:

(i) easily define and control the variable resolution settings: chopper speed and phase and if possible (self) solve specific bugs or red-flag runs.

(ii) easily define and control the variable parameters: **counting time** (that should all be self-adjustable, see next slide), T, magnetic and electrical field (or voltage), pressure, humidity, laser pump.

(iii) sequentially change the run process also providing for flexibility for adjustments

(iv) send warnings!

Display in cabin

- proposal number, run numbers, set run time, time left
- 2D of all monitors and detectors: rates
- wavelengths (set, actual, band)
- shutter, motor, chopper (freq+phase, locked), slit posn; SE parameters
- vacuum, cooling status
- integrated on all time channels or early, middle, late?
- operation mode (high res, high flux)
- separate screen for ESS values: power, current, etc., run status? PPS status for beamline?

Automated post-processing: The software should also allow for data reduction and quick analysis method. Therefore, one needs to be able to:

(i) ability to share certain files between users (resolution)

(ii) include the reduction/analysis when setting a series of new scans or modify an existing series.

(iii) easily visualise/review a series of runs/scans/automated fits to check if they worked well

(iv) change the reduction process as well as the fitting procedure in the sequence of scans or runs on-going

(v) easily extract the fitting parameters (i.e in a txt or excel file)