



Nerthus is a Germanic Mother Earth goddess. Some identified her with the god Njörd, with whom she might form a deity pair.

NERTHUS: NEutRon THERmal time-focUssing Spectrometer

A new instrument for the ESS proposed by Mo Aouane, Christian Balz, Daria Noferini, Andrea Orecchini, Francesco Sacchetti, and Marco Zanatta.



EUROPEAN
SPALLATION
SOURCE



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UNIVERSITÀ DEGLI STUDI
DI PERUGIA



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DI TRENTO

ESS Spectroscopy STAP 21/04/2026

Why NERTHUS?

The First (pseudo) Brillouin zone gap

Dispersion curves and lifetime of coherent excitations in amorphous and crystalline powder materials
(biological function in biomolecules, transport properties in energy materials, magnetic interactions in novel magnetic materials...)



Access to the 1st (pseudo) Brillouin zone



Thermal exchanged energies and low Q (0.1 \AA)

Difficult region!

Why NERTHUS?

The First (pseudo) Brillouin zone gap



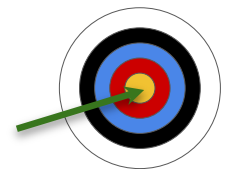
neutron Brillouin scattering (NBS) requirements:
thermal incident energies, small-angle detection, low divergence,
low background, high flux

Dedicated instrument: BRISP@ILL (decommissioned)
- high background due to location
- not very versatile

Special configuration at different spectrometers
- require aggressive collimation paid in low flux
- more versatility

NERTHUS

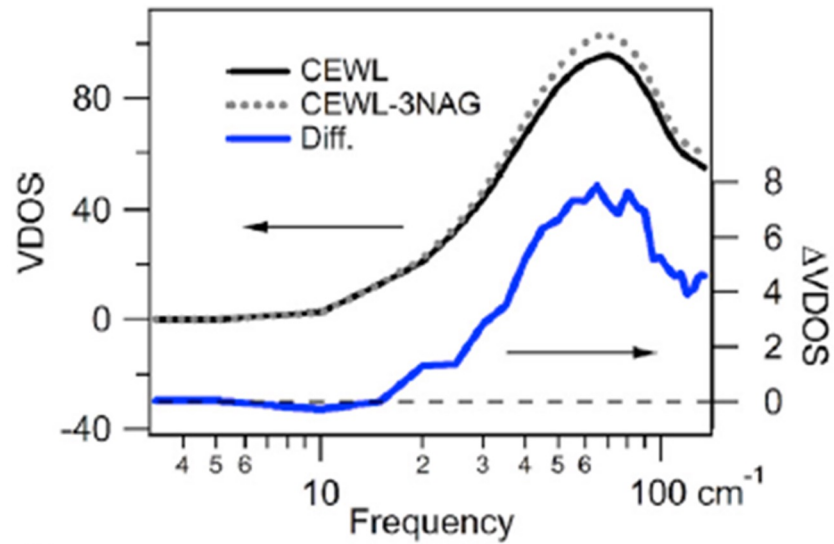
Optimised for Brillouin, with large angle option → versatility, combination with GDOS
Using the strengths given by time focussing opportunities at the ESS to achieve a
combination of **high flux** (allowing polarisation analysis) and **low background** never
reached before in the NBS region → **new scientific possibilities**



Science cases

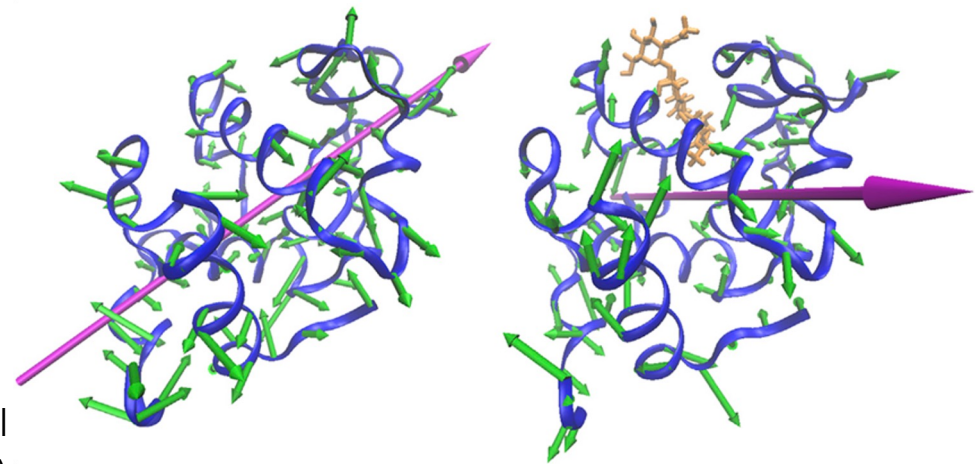
The role of collective modes in **protein functionality**
(e.g. Lysozyme)

Life science



A tiny difference in the neutron VDOS of Lysozyme...

...is due to one specific type of functional
collective modes (directionality)

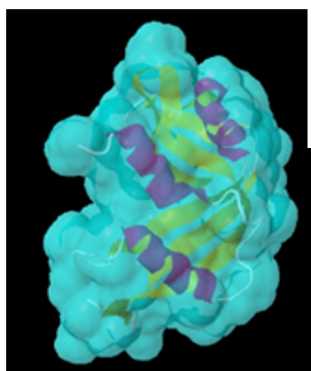


Niessen, Paciaroni, Orecchini et al., *Biophys. J.* 112, 933 (2017)

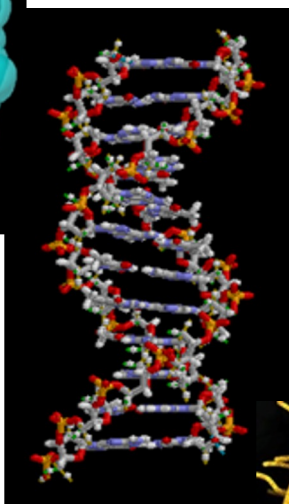
Science cases

Collective modes in **hydration water** of biological systems of increasing complexity

Life science



Ribonuclease A

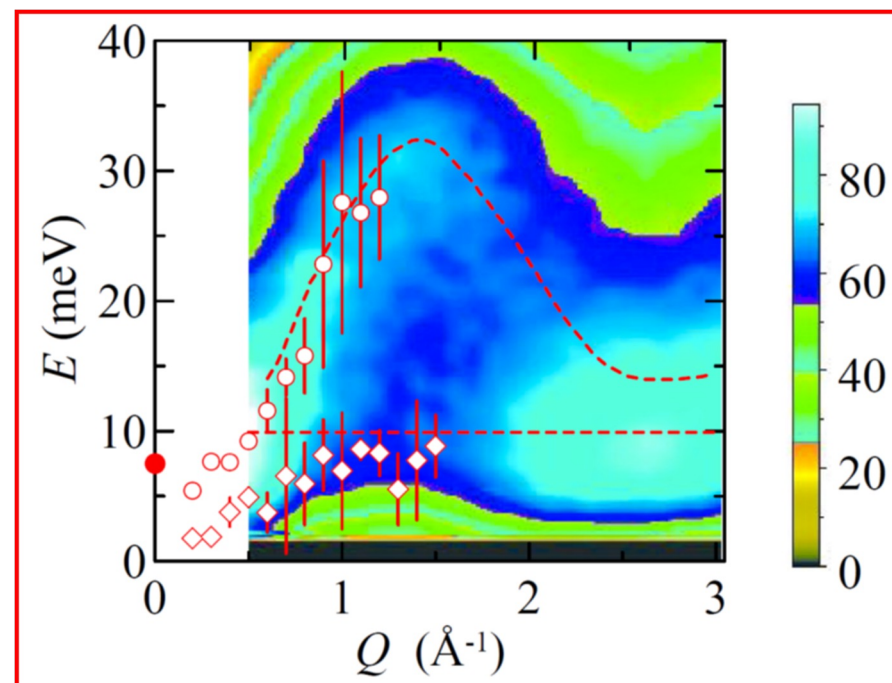


DNA

Escherichia coli



Data vs Simulations

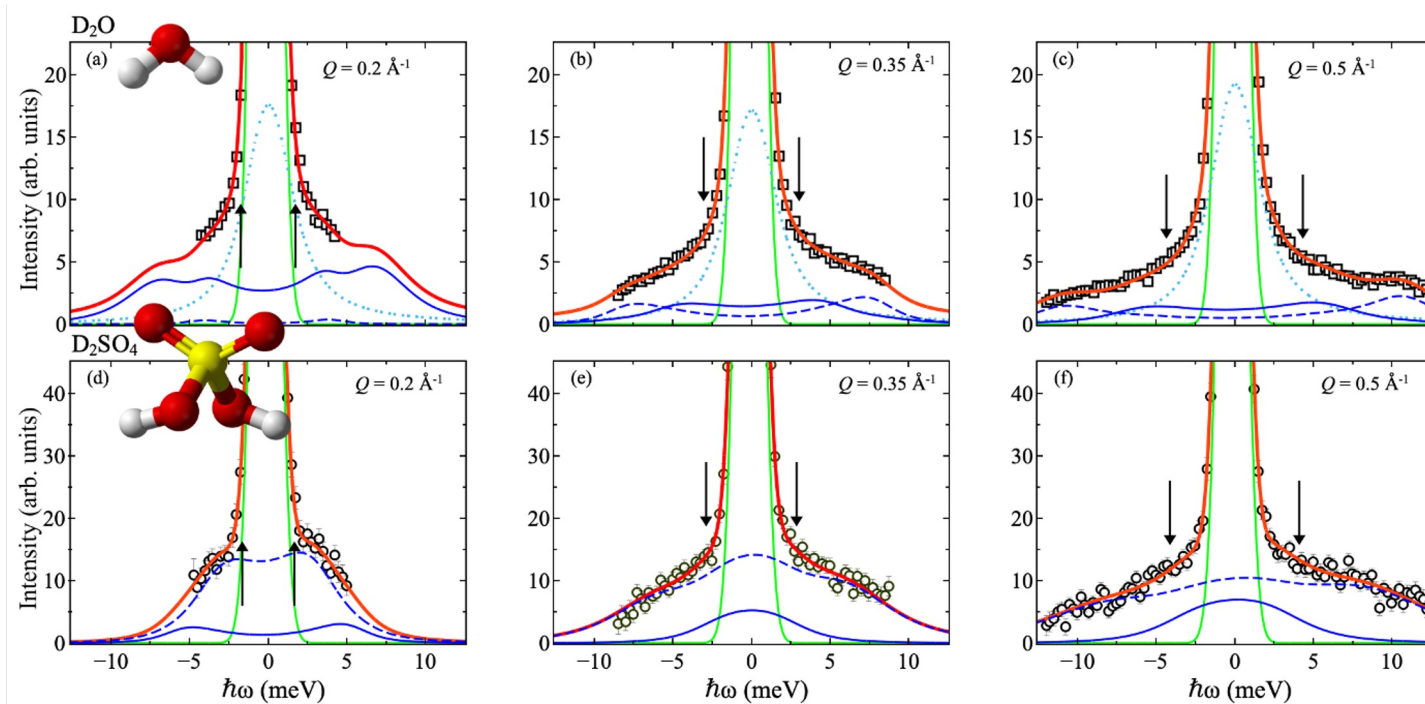


Orecchini, Paciaroni et al., JACS, 131, 4664 (2009)

Science cases

Complex pattern of collective excitations in **liquids** and **disordered materials**.

Liquids & disordered materials



Collective dynamics in molecular liquids
(es. water and sulphuric acid)

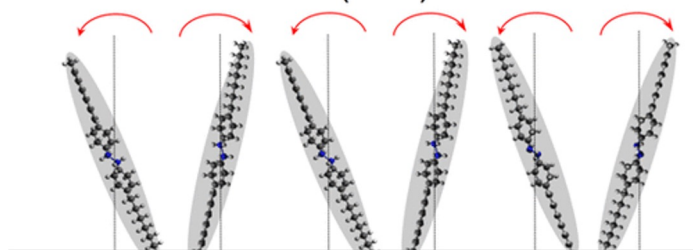
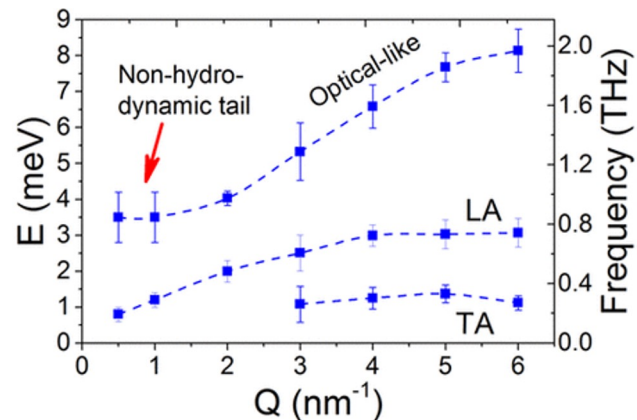
Theory: a single longitudinal acoustic mode, strongly damped.

Experiments: at least two modes (interacting).

The simultaneous study of collective modes and DOS on the same sample can elucidate the nature of the excitations.

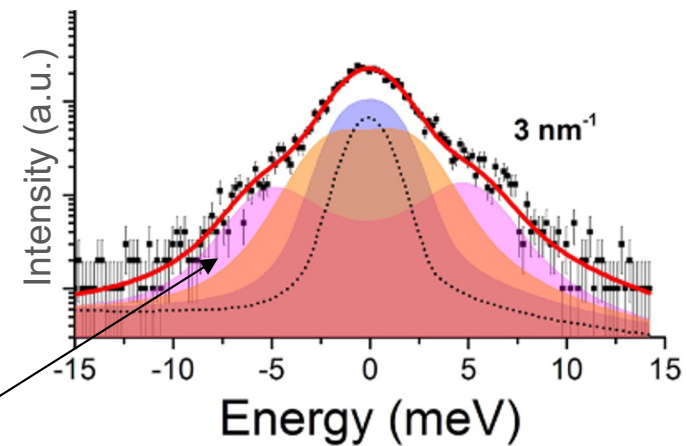
Zanatta et al. J. Mol. Liq. **393**, 123550 (2024)

Science cases



Optical phonon in the smectic phase (out of phase tilts of the aligned liquid crystals) → engineering optically active crystals

Liquid Crystals



IXS → limited energy resolution, not able to fully resolve the individual phonon modes

Bolmatov et al, Nano Lett. 2017, 17, 6, 3870–3876

Science cases

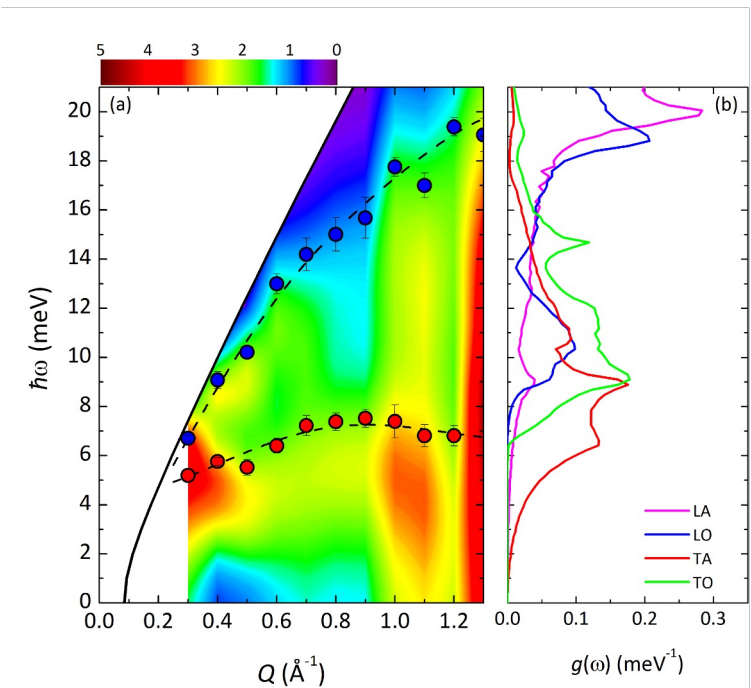
Liquid state: molten salts and liquid metals

Applications in concentrated solar power, grid-scale batteries, generation IV nuclear reactors and fusion reactor concepts.



High-frequency density fluctuations and phonon-like modes
→ thermal conductivity, viscosity, ion transport, stability

Energy materials



Zanatta et al., PRL 114, 187801 (2015)

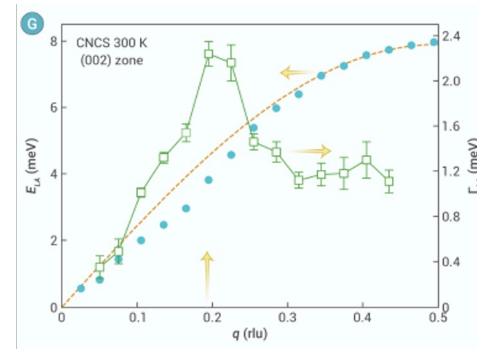
Science cases

Energy materials

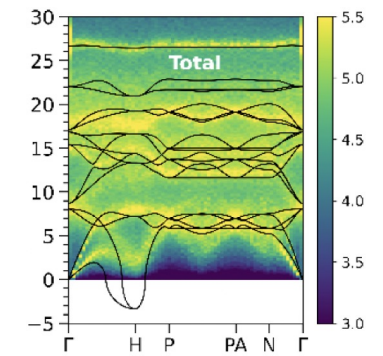
Solid state: thermoelectrics for waste heat recovery, **superionic conductors** for all-solid-state batteries, **hydrogenated materials** for solid-state fuel cells and solid-state storage

- Lattice dynamics strongly linked to performance in energy applications
- Difficult to isolate collective excitations from strong incoherent signals
- Difficult to obtain (large) single crystals for newly developed materials

Nerthus → better access to low-Q regions and combination with polarisation analysis

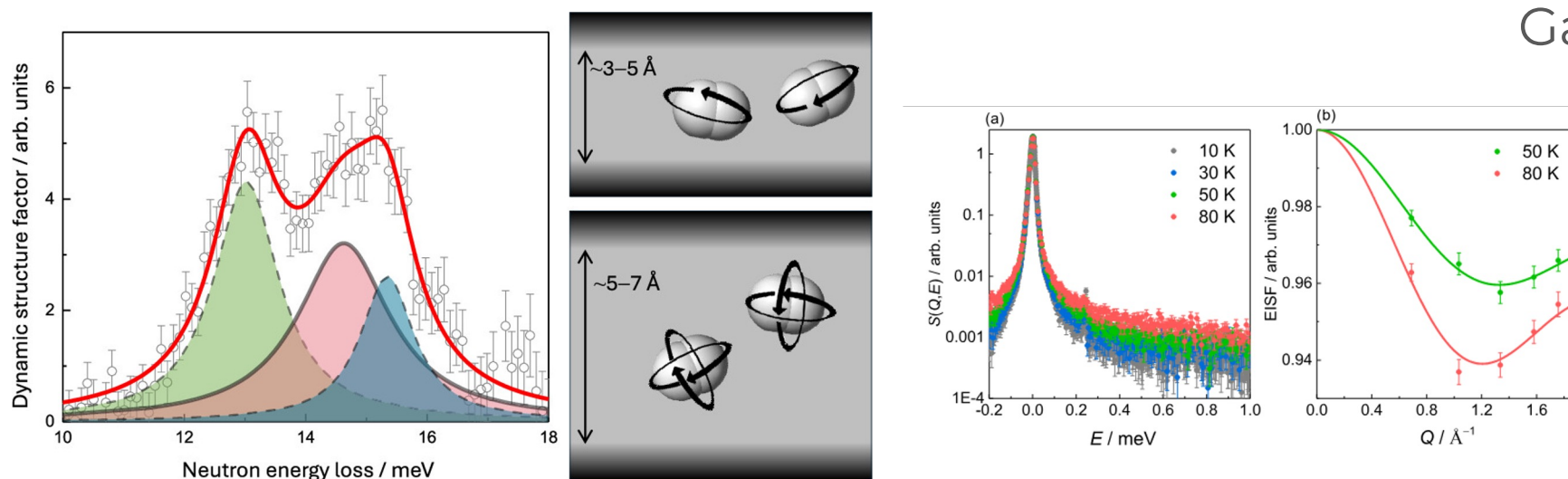


Zhu et al. *The Innovation Energy* 1(4):2024



Gupta, et al. *Chemistry of Materials* 2024

Science cases



Gas sorption

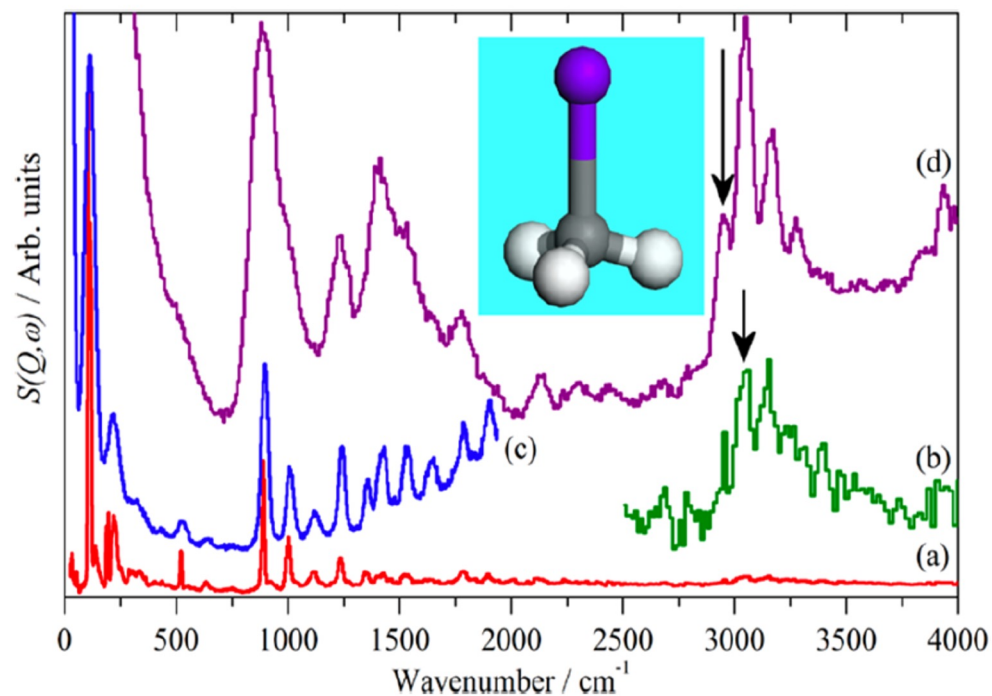
Restricted Dynamics and Para-Ortho Conversion of H₂ Adsorbed in Micro- and Mesoporous Carbide-Derived Carbon: A Quasi- and Inelastic Neutron Scattering Study

Miriam Koppel, Rasmus Palm,* Riinu Härmas, Mark T. F. Telling, Manh Duc Le, Tatiana Guidi, Kenneth Tuul, Maarja Paalo, and Enn Lust

- H₂ confined inside porous carbon materials: Interest from a QENS and INS perspective
- in-situ investigation of the p-o transition and the EISF to determine the confining geometry and H₂ mobility (adding capacity to T-REX)

Science cases

Catalysis



Measurement on Iodomethane at 10 K

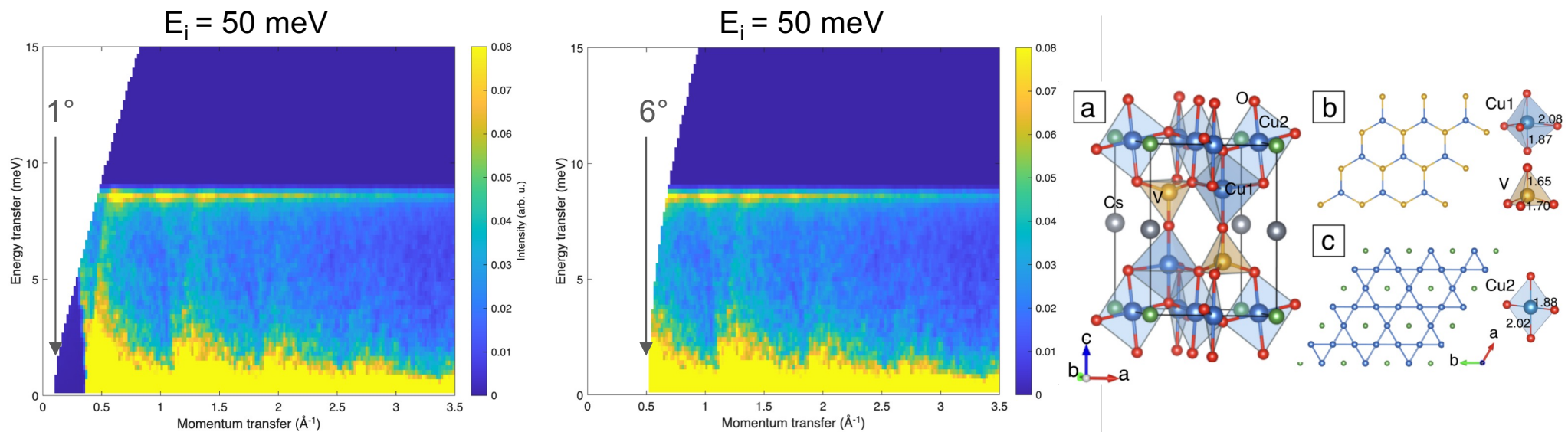
- a): TOSCA
- b): TOSCA x10
- c): MAPS - $E_i = 250\text{meV}$
- d): MAPS - $E_i = 600\text{meV}$

- Capacity: Complementarity with VESPA measurements
- New capability: Homogeneous catalysis in liquid phase \leftarrow low Q values; in-situ, high temperature, processes \leftarrow low background

Science cases

Magnetism

Low-Q magnetic excitations of ferromagnetic powders



- Simulated powder spectrum of Averievite, featuring coupled Cu Kagome layers in a complex 3D structure with a mixture of ferromagnetic and antiferromagnetic exchanges.
- One simulation is for a minimum scattering angle of 1 degree (NERTHUS) and the other one for 6 degrees (typical direct geometry ToF spectrometer).

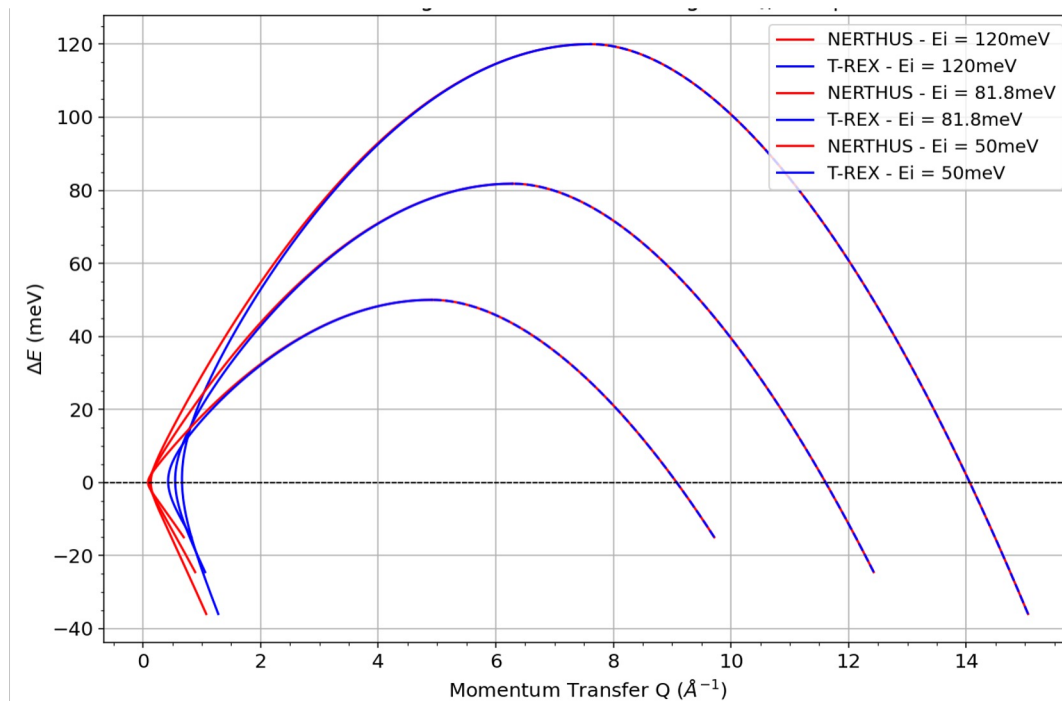
Preliminary Instrument Concept

The science case requires:

- high versatility in the thermal range;
- small scattering angle;
- good energy resolution;
- high flux & low background;
- polarization analysis;

neutron energy	E	20 meV ÷ 127 meV
energy resolution	$\Delta E/E$	~ 3%
min scattering angle	θ_{\min}	~ 1°
max scattering angle	θ_{\max}	~ 130°

Instrument requirements

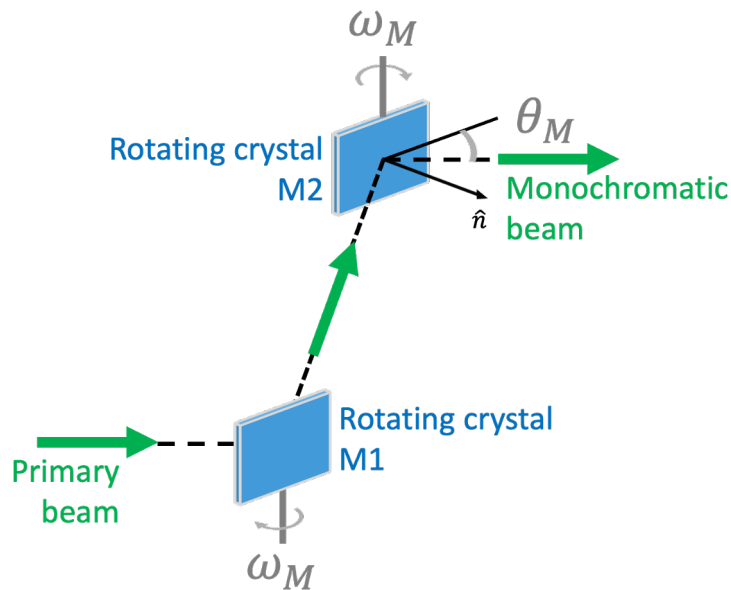


Direct geometry thermal neutron spectrometer based on time-focusing with DRCM.

Preliminary Instrument Concept

Time-focussing with DRCM

The use of a **double rotating crystal monochromator** (DRCM) allows the implementation of time-focusing without increasing the beam divergence.

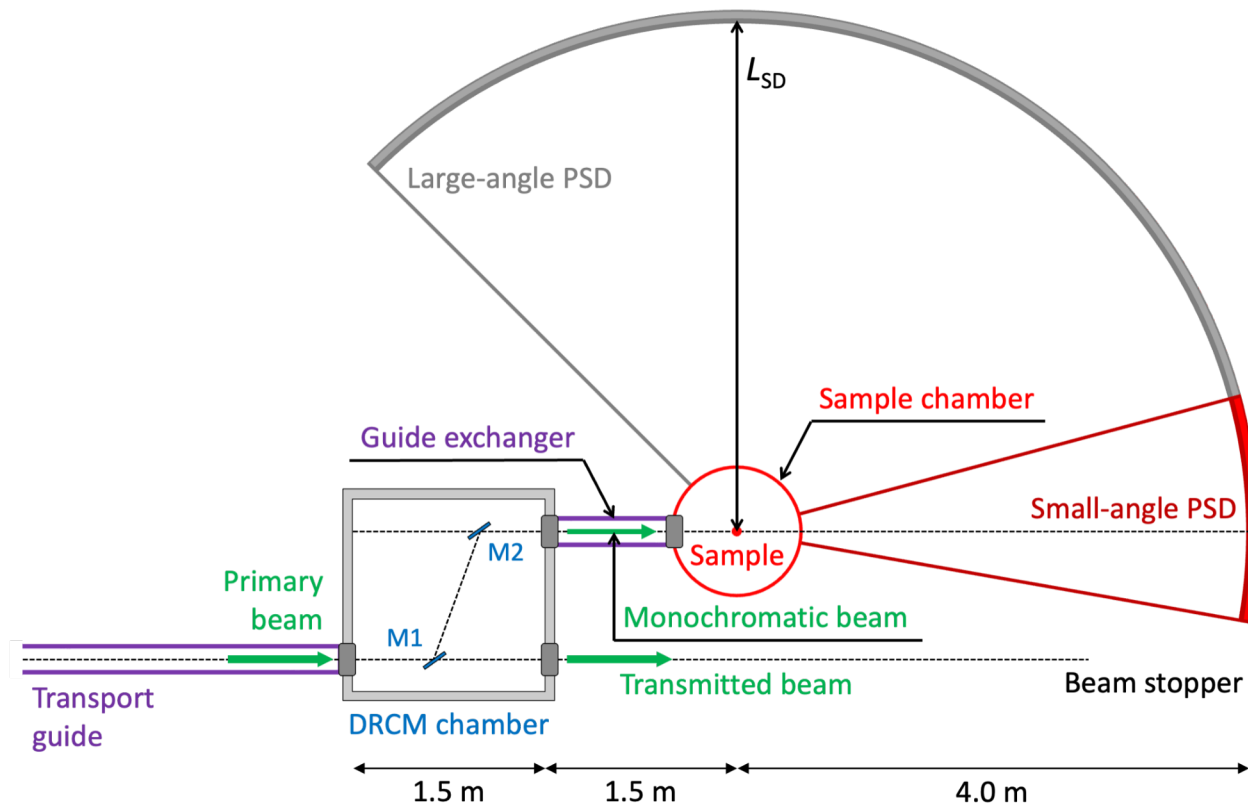


M1 and **M2** rotate at an angular speed ω_M and continuously sweeps the Bragg angle θ_M

- The DRCM extracts a **broad wavelength band** from the primary beam into a monochromatic one.
- The DRCM crystals are in parallel configuration so the **divergence is conserved** from the primary beam in the monochromatic one.
- The DRCM rotation direction allows slowest and fastest neutrons to match the **time-focusing condition** at the detector thus preserving the energy resolution.
- The DRCM decouples the primary and the monochromatic beam with a **reduction of the background noise**.

Preliminary Instrument Concept

Proposed design



Transport guide

- can be relatively short and straight.

DRCM

- can select different wavelengths with different resolutions;
- can be used in cascade thus allowing multiplexing;
- decouples the primary and monochromatic beam.

Guide exchanger and sample chamber

- fit polarization analysis;
- fit optics and sample environment.

Small angle detector (for BNS)

- is a PSD detector from -10° up to 15° .

Large angle detector (for INS)

- is a PSD detector from -10° up to 135° .

Preliminary Instrument Concept

Expected performance

We carried out **detailed analytical calculations** of energy resolution ΔE , momentum resolution ΔQ and gain to a chopper spectrometer G .

M. Zanatta, K.H. Andersen, P.P. Deen, A. Orecchini, A. Paciaroni, C. Petrillo, and F. Sacchetti, Rev. Sci. Instrum. **90**, 095101 (2019)

DRCM crystal	n	λ_j (Å)	E_i (meV)	θ_M (°)	ν_M (Hz)	$\Delta E_i/E_i$ (%)	G
Cu(220)	2	0.80	127.81	38.75	105	2.0	21.0
Cu(220)	2	0.90	100.99	44.77	105	2.0	21.6
Ge(355)	2	0.80	127.81	47.05	147	3.1	12.9
Ge(355)	2	0.90	100.99	55.43	147	2.9	12.1
HOPG(002)	4	1.00	81.80	36.61	84	3.3	12.4
HOPG(002)	2	2.00	20.45	36.61	42	3.3	12.4

TF spectrometer

$$I_{TF} = \Phi(E_i) T_G S_M R^2 \nu_M \Delta T \Delta \Omega_M \Delta E_M$$

Chopper spectrometer

$$I_{CS} = \Phi(E_i) T_G S_C T_C \nu_C \Delta t \Delta \Omega_C \Delta E_C$$

Gain factor G

$$G \sim \Delta T / \Delta t$$

Preliminary Instrument Concept

Risks and mitigations (1)

The DRCM is the innovative component of NERTHUS.

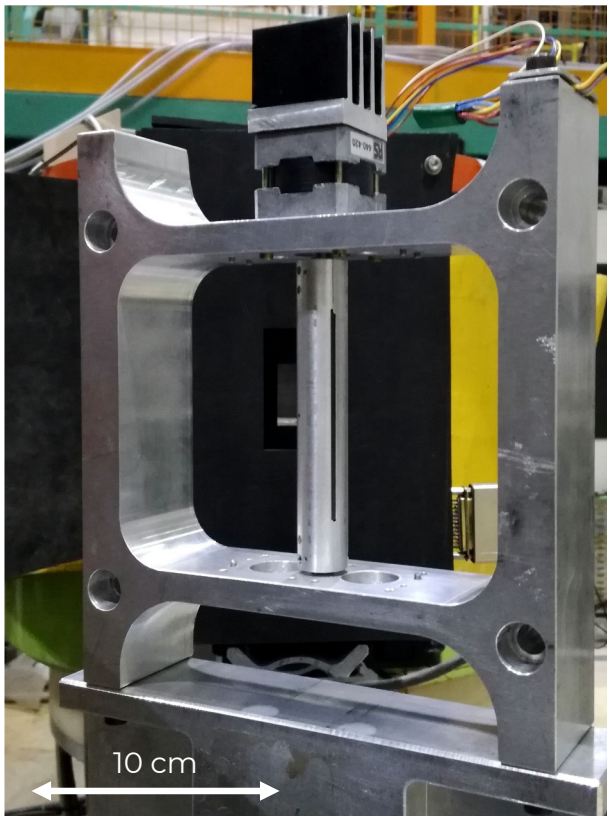
DRCM rotating element: cylinder composed by **two symmetric halves** (diameter 2 cm), **slab-shaped crystals** lay on the cylinder axis; the sample holder is in aluminum and most of the inner material is removed (external wall <1 mm).

State-of-the-art

- We built several prototypes of DRCM.
- We tested the rotating element at T13A@ILL and IN3@ILL.
- We tested the DRCM at IN3@ILL and G4.3@LLB.
- We did long term mechanical tests at 100 Hz (several months).

Risk mitigation

- The DRCM can be validated at the ESS test beamline.



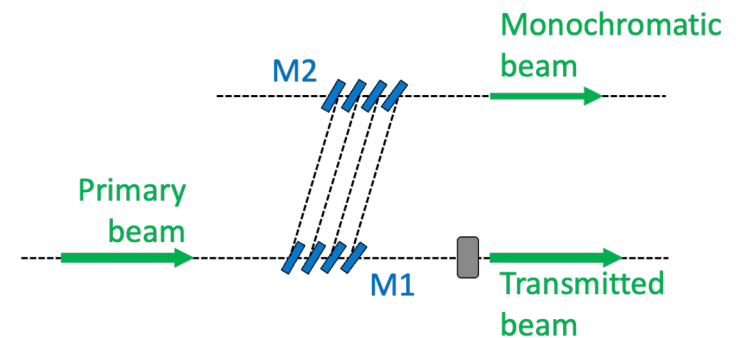
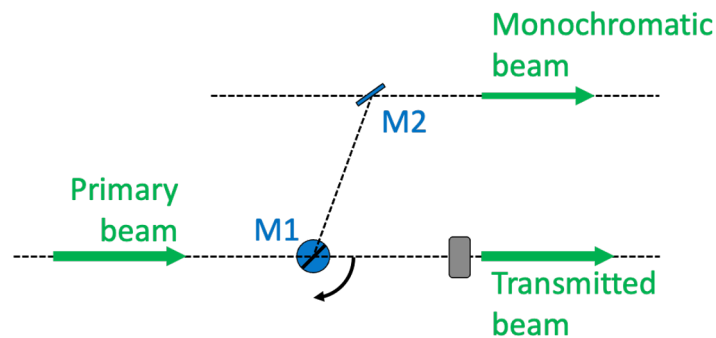
M. Zanatta *et al.*, J. Phys.: Conf. Ser. **746**, 012002 (2016).

Preliminary Instrument Concept

Risks and mitigations (2)

Risk mitigation

- Explore further possible double-crystal based configurations to get time-focusing.
 - Broad wavelength band extraction with time-focusing.
 - Double crystals configuration to separate the primary and monochromatic beam.
 - Parallel crystals configuration to conserve the divergence.



Hybrid double crystal configuration

- M1: rotating crystal(s) monochromator.
- M2: static crystal monochromator.

Static double crystal configuration

- M1: cascade of crystal monochromators.
- M2: cascade of crystal monochromators.

Preliminary Instrument Concept

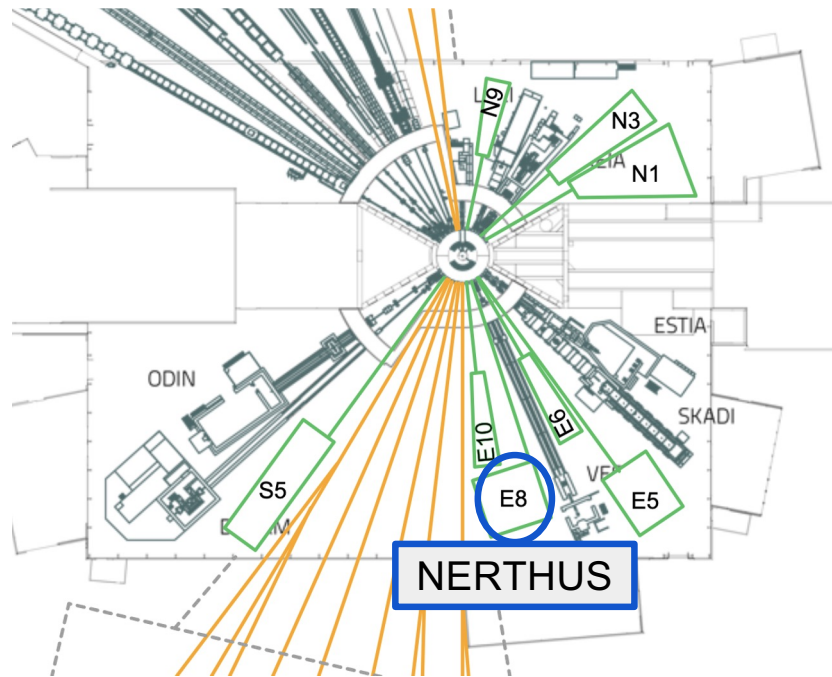
Sample environment

Sample environment area to ensure versatility for different scientific needs. Requirement for PA is low magnetic permeability (previous experience on 1st suite instruments).

- **Cryofurnace:** T range 2–800 K (standard for most science cases)
- Access to **high temperature furnace:** T range 300 –1300 K (inorganic glasses, energy materials...)
- Access to **high-pressure systems** (Paris-Edinburgh cells, liquid pressure cells, gas pressure cells) and **gas sorption equipment**.
- Rotation stage, for single crystals

Preliminary Instrument Concept

Proposed location and lab access



Compact instrument, it could fit in many locations, and even symbiotic for Njörd, with some adaptations to be considered.

Beamport E8 maximise the thermal extraction and allows sufficient space for the large detector option.

Several laboratories with different complementary characterisation techniques can be accessed in the different buildings.

Thank you!

