Spectroscopy Division

Science Away Day 2024

PRESENTED BY PASCALE DEEN

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European Spallation Source (ESS), ERIC, Sweden.
Affiliate Professor in Solid state Physics and Neutron Scattering
Niels Bohr Institute, University of Copenhagen
H-index 27 (Scopus), i10 index 45, 3295 citations; 78 peer reviewed publications (2024)
ORC-ID: 0000-0002-0204-0802

Technical Research Profile: Neutron instrumentation focussed on neutron spectroscopy and neutron polarisation analysis.

Scientific Research Profile : Strongly correlated magnetism, Magnetic Frustration, Quantum magnetism.

2003 - 2006 Post-doctoral Fellow: European Synchrotron Radiation Facility, Grenoble, France: High pressure techniques for Resonant X-ray Magnetic Scattering in strongly correlated magnetism.

2006 - 2011 Instrument Scientist: Institut Laue Langevin, D7, Grenoble, France.

2011 - 2015 Scientist for Spectroscopy: European Spallation Source.

2012 - 2023 Adjunct Associate Professor: University of Copenhagen

2015 - 2021 Lead scientist for CSPEC, ESS

2021 - 2023 Senior Scientist for Spectroscopy, European Spallation Source.

Aim of the spectroscopy division

Drive towards science

The spectroscopy division, within the science directorate, was recently formed (February 2024) and the aim of the division is to:

(1) Support NSS in the construction of the spectroscopy instruments within the first instrument group (MIRACLES/CSPEC/BIFROST/TREX/VESPA).

(2) Ensure scientific excellence and world leading performance on these instruments and their associated sample environment and laboratory requirements. (& In-kind partners)

(3) Operate, maintain & upgrade the neutron instruments.

(4) Develop a scientific culture in which the users are able to acquire the required support. and developments needed to drive scientific excellence.

(5) Develop the instrument suite beyond the first 15.

Spectroscopy: Measuring dynamics of materials S(**Q**,ω) : functionality. Ordered phase of $Bi_2Fe_4O_9$

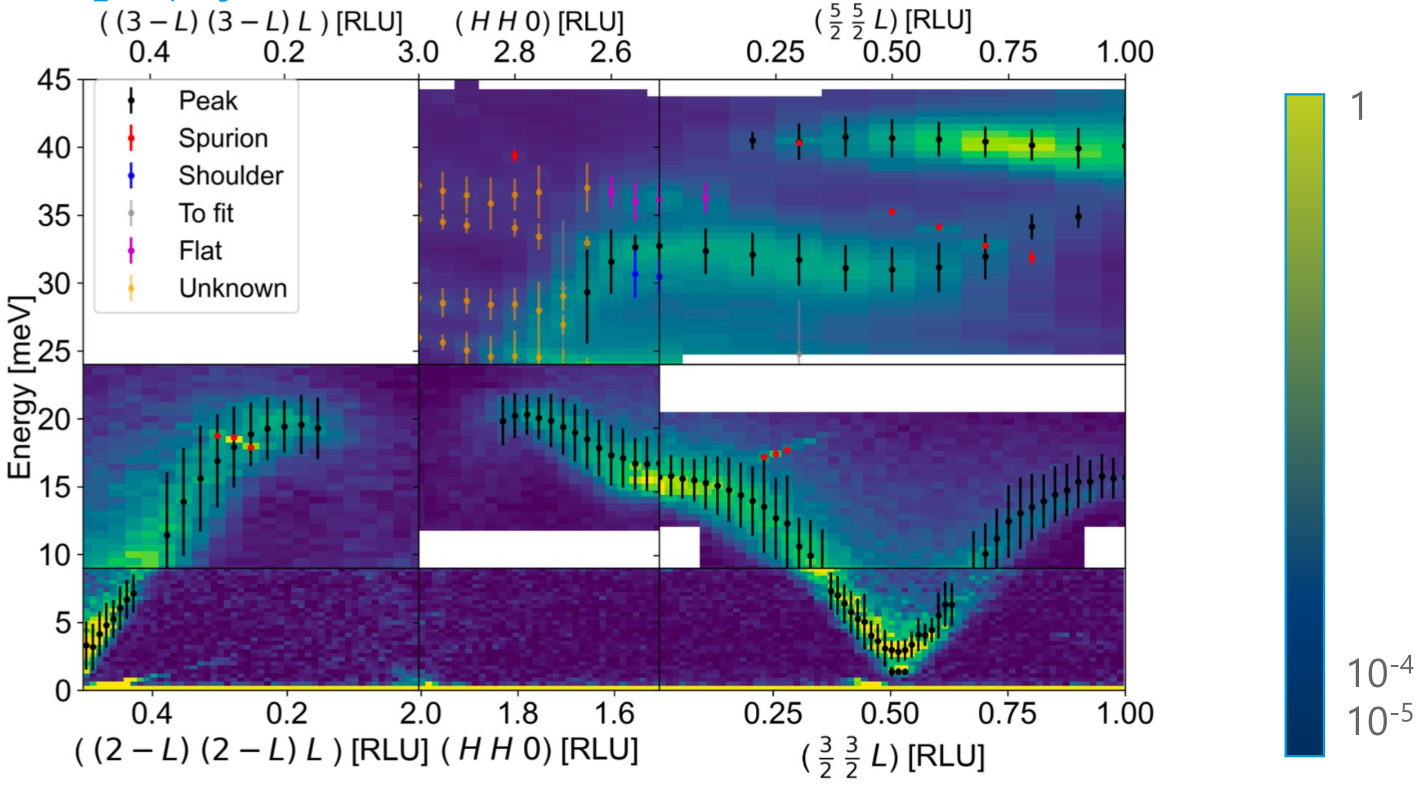
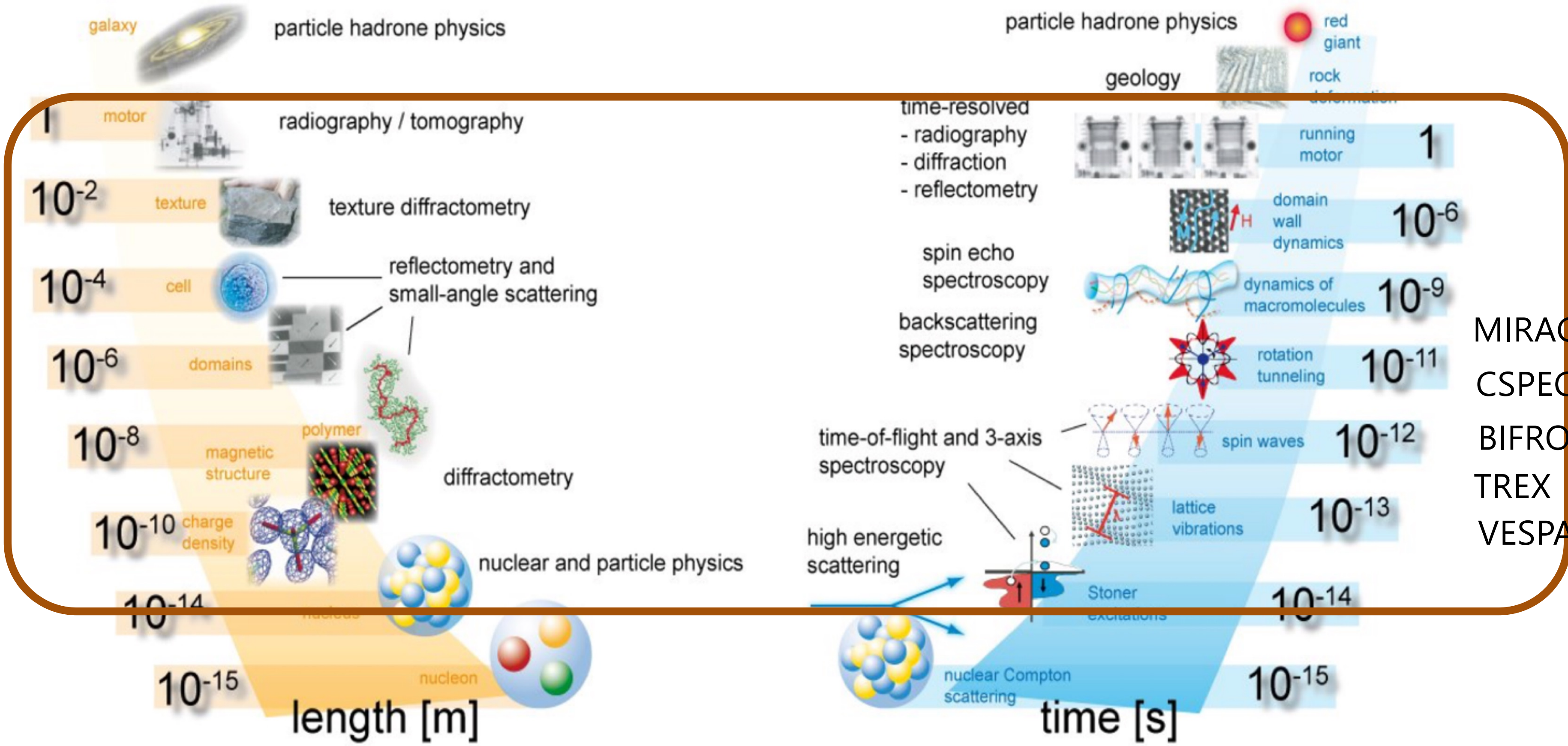


Figure 48: All data in one QE-plot, from CAMEA (0-9 meV), EIGER (9-24 meV) and IN20 (24-45 me
The fitted data is shown on top; mean μ and standard deviation σ.

- Weak signals – 10^{-4} 10^{-5}
- Broad features in S(**Q**,ω)

Accessing materials properties by neutron perturbation

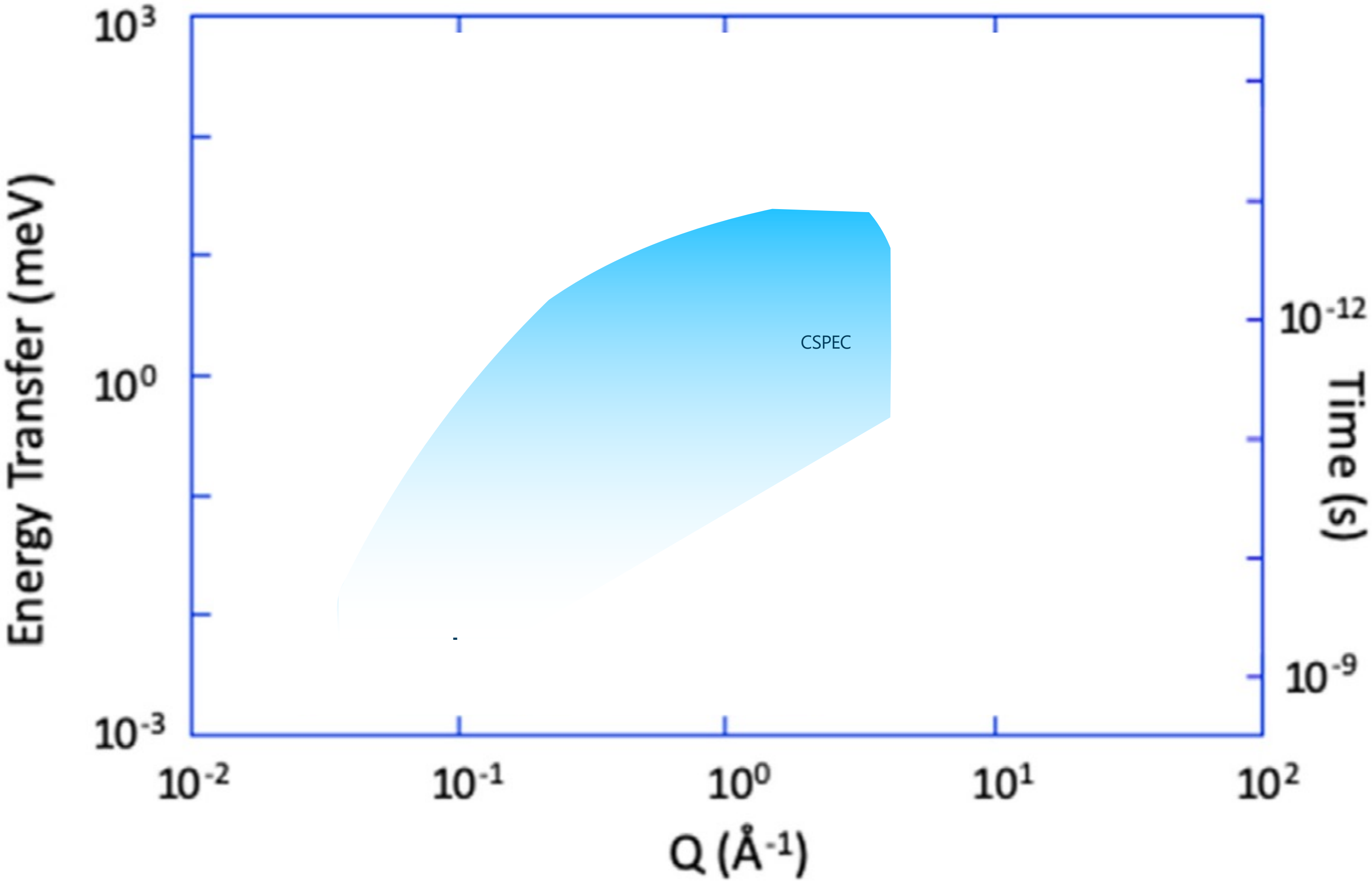
T = 293 K, 25.2 meV, 1.798 Å



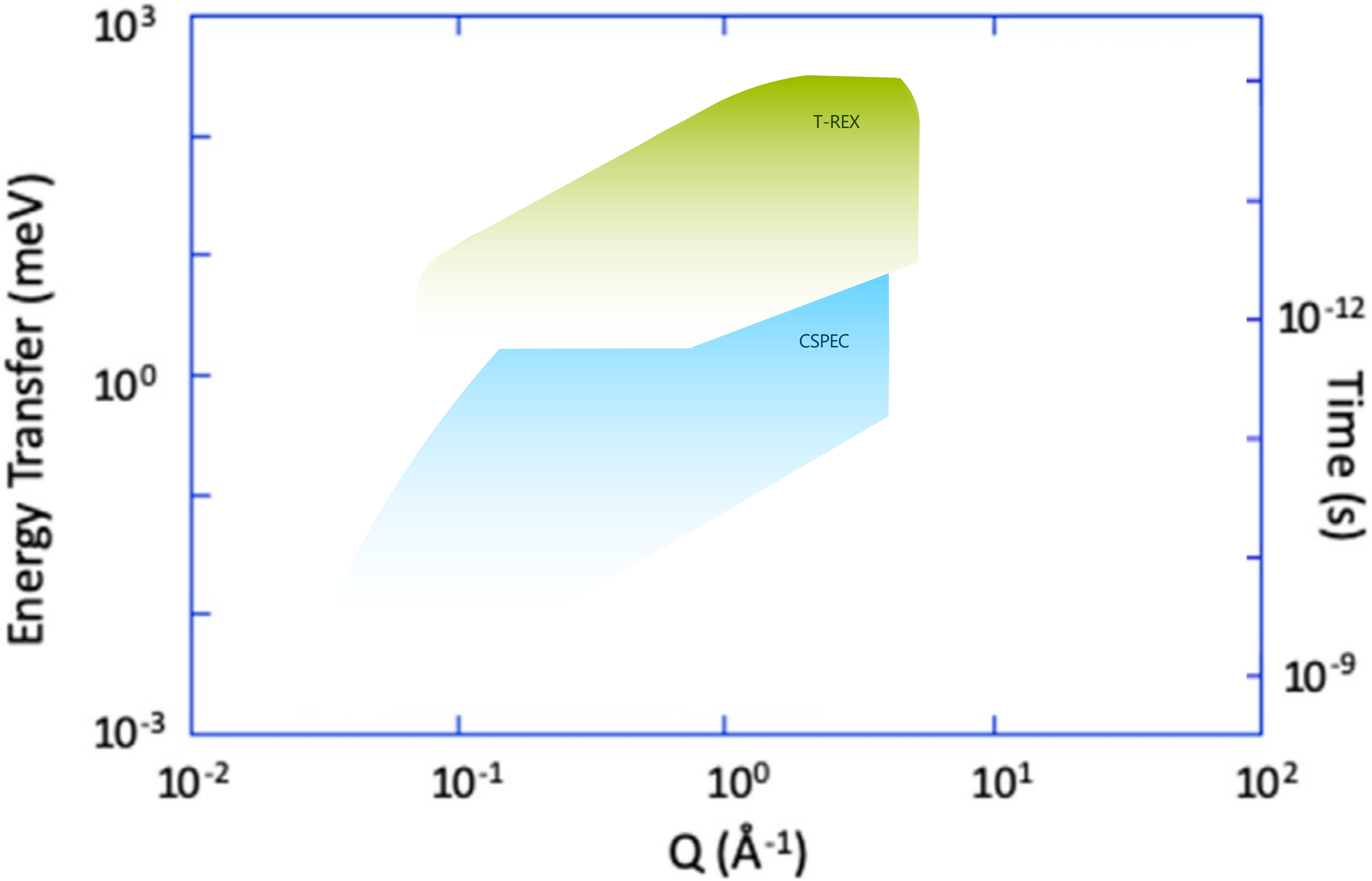
MIRACLES
CSPEC
BIFROST
TREX
VESPA.

Different length and time scales, that can be measured with the various instruments (Picture: Karin Griewatsch, Kiel University, KFN).

Spectroscopy suite - covers a broad range of time and spatial scales

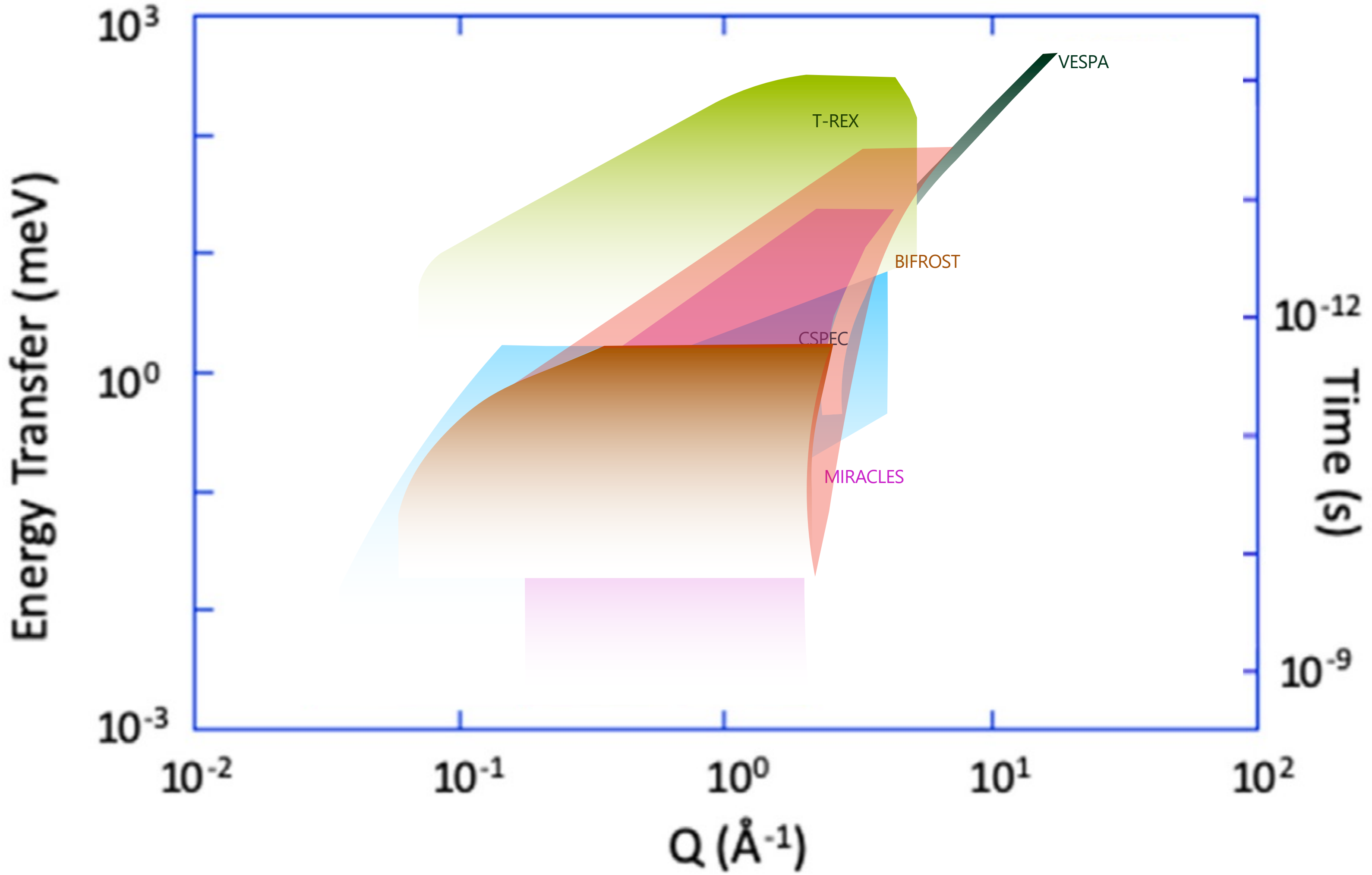


Spectroscopy suite - covers a broad range of time and spatial scales

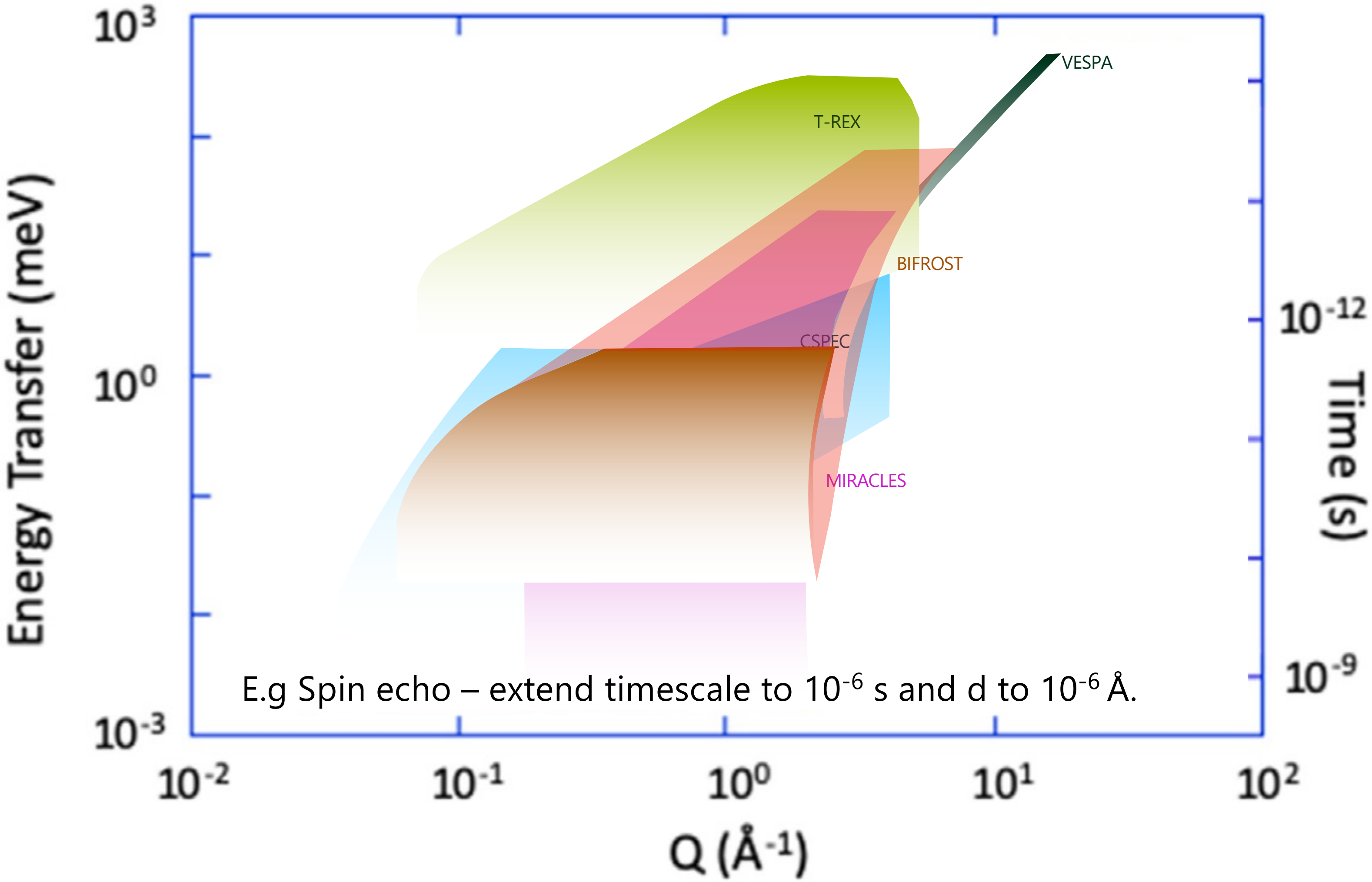


Spectroscopy suite - covers a broad range of time and spatial scales

More needed



Spectroscopy suite - covers a broad range of time and spatial scales



E.g Spin echo – extend timescale to 10^{-6} s and d to 10^{-6} Å.

Spectroscopy

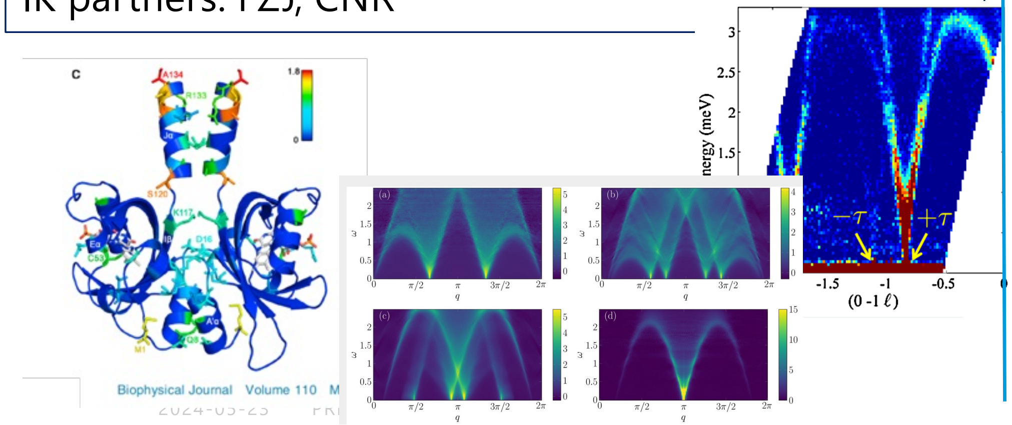
5 Instruments

Direct-Geometry Spectroscopy

General-purpose chopper spectrometers

CSPEC: Cold chopper spectrometer
Scientist: Daria Noferini (ESS), Pascale Deen (ESS)
IK partners: TUM, LLB

T-REX: Bispectral polarised chopper spectrometer
Scientist: Christian Franz (FZJ), Scientist (ESS)
IK partners: FZJ, CNR



Indirect-Geometry Spectroscopy

Crystal-analyser instruments

MIRACLES: Backscattering spectroscopy
Scientist: Felix Villacorta (ESS-Bilbao), Jose Pereira (ESS-Bilboa), Scientist (ESS)
IK partners: ESS-Bilbao, KU

BIFROST: Single-crystal extreme spectroscopy
Scientist: Rasmus Toft-Petersen (DTU)
IK partners: DK, PSI, LLB, IFE, Wigner

VESPA: Vibrational spectroscopy
Scientist: Adrien Perrichon
IK partners: CNR, ISIS

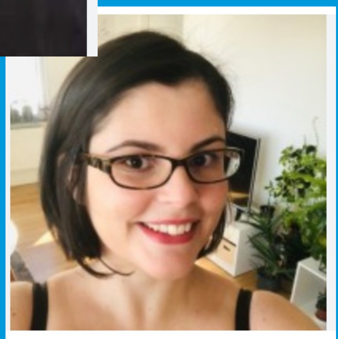
Staff in Spectroscopy Division

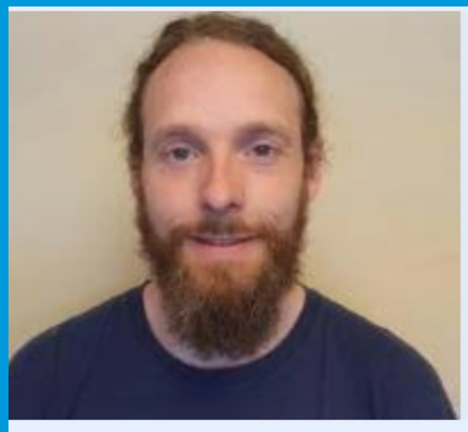
Instrument	Instrument scientists	Lead engineer	Instrument operational engineer	DMSC	Place of work	TG5
MIRACLES	Felix Villacorta ***Recruit @ESS***	Alex Conde Estebanez		Henrik Jacobsen	Spain	Q1/27
CSPEC	Daria Noferini, Pascale Deen	Fernando Moreira		Greg Tucker/Henrik Jacobsen	ESS	Q1/27
BIFROST	Rasmus Toft-Peterson	Liam Whitelegg (50%)	Tamires Gallo	Greg Tucker	ESS	Q2/25
TREX	Christian Franz **Recruit @ESS**	Marcel Serwe			Julich	Q2/27
VESPA since 04/2024	Adrien Perrichon	Liam Whitelegg (50%)			ESS	Q4/27

Table 1: Spectroscopy instruments, their respective principal staff members, place of work and approximate TG5 date.

Spectroscopy Division

Science Away Day 2024





ESS: a source to deliver meV neutron for the study of materials

Neutrons probes directly **magnetic spins**.

High technology society: magnetic and electronic phenomena.

Magnetic spins:

- quantum computing / Classical

  = 200 sec/10 000 years (Google 2021)

- Superconductivity : lossless power transfer

- Magnetocaloric cooling : low carbon

The Nobel Prize in Physics 2016

David J. Thouless, F. Duncan M. Haldane and J. Michael Kosterlitz
"for theoretical discoveries of topological phase transitions and topological phases of matter"

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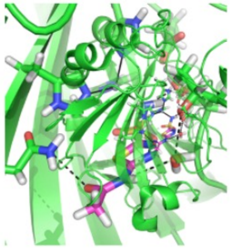
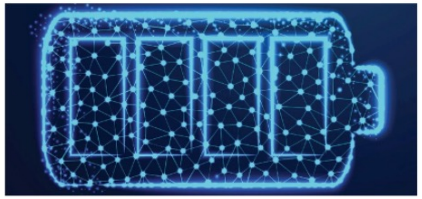
Neutrons: Probes directly light elements

(hydrogen, lithium)





- Biological processes: where hydrogen (H) atoms are and how they are transferred between biomacromolecules, solvent molecules, and substrates.
- Optimise diffusion in battery materials.

The Nobel Prize in Chemistry 2019

John B. Goodenough, M. Stanley Whittingham and Akira Yoshino "for the development of lithium-ion batteries"

NSS high level schedule

With T2T3 replanning

TG5 = instrument ready for hot commisioning

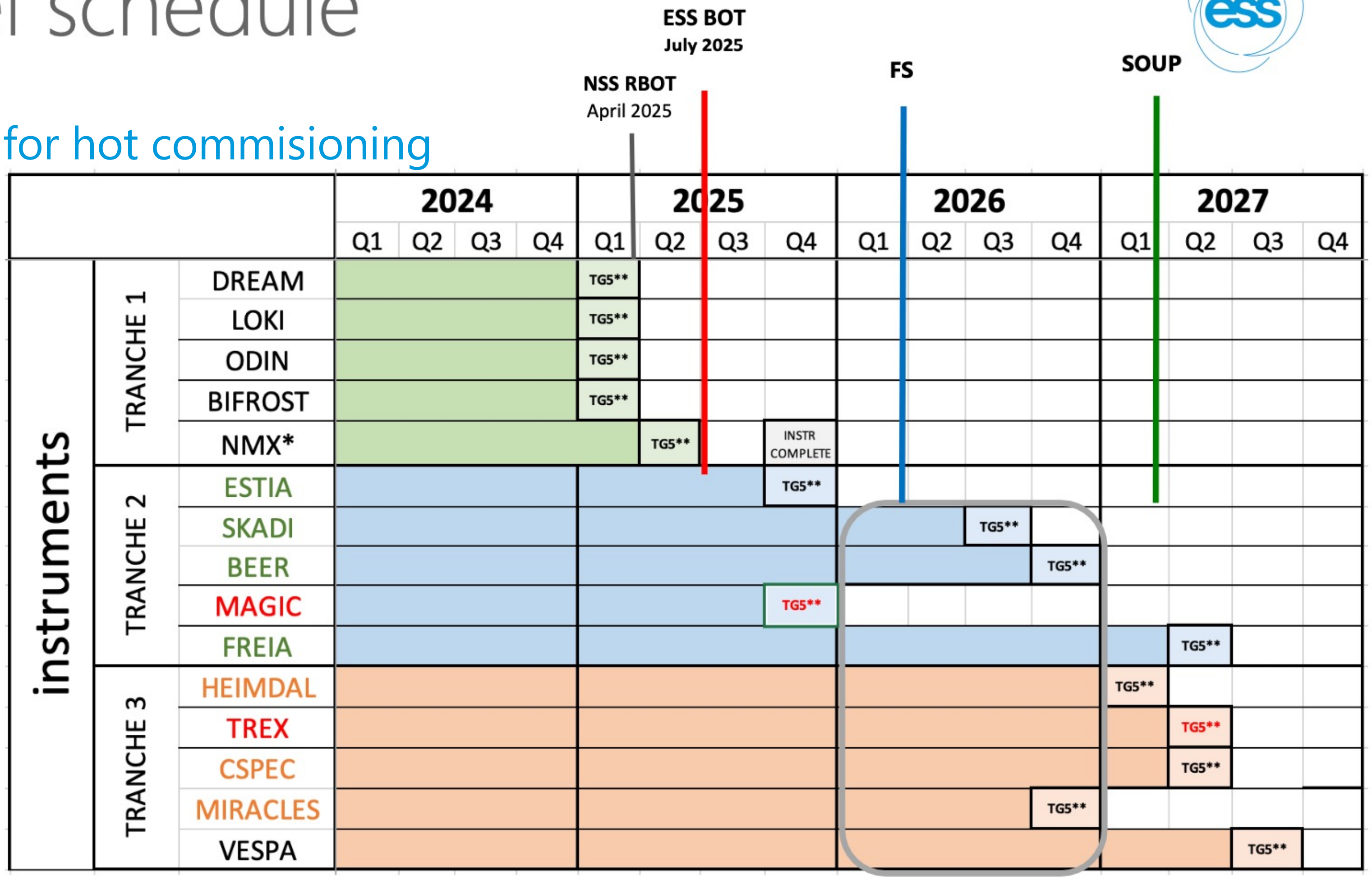
NSS “end of project” defined as TG5 for instrument 15

TG5 milestone (IK partner) is followed by Instrument SRR (NSS responsibility), which triggers Hot Commissioning (Science).

NSS is currently tracking **4-5 instruments passed Safety Readiness Review (SRR)** at the point of **BOT.**

T2T3 replanning ongoing:

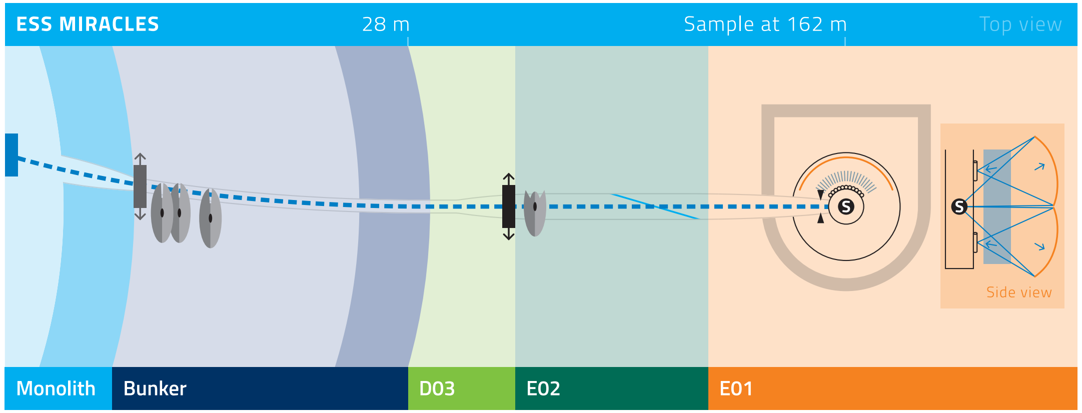
Green = almost ready
Orange = ongoing (draft dates)
Red = not started (draft dates)



Instrument Details

MIRACLES

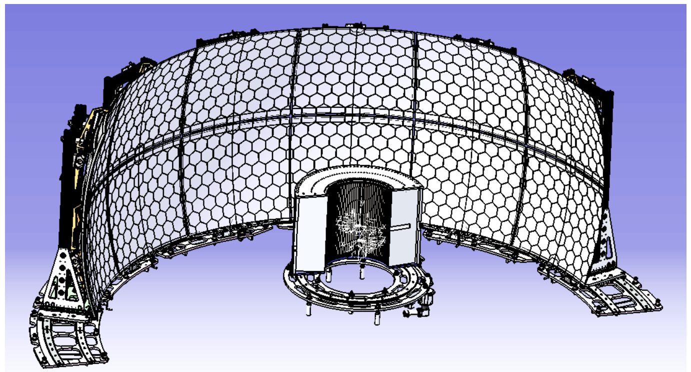
Backscattering Spectrometer



- **Life sciences**: degenerative diseases, protein dynamics and enzyme catalysis
- **Pharmaceutical studies:** drug delivery.
- **Energy sciences:** catalysis, fuel cells and H2 storage, CO2 capture, proton diffusion.
- **Polymer sciences:** organic electronic devices, viscoelasticity.
- **Climate change:** waste containment, ice formation, Portland-alternative cements.
- **Magnetic materials:** molecular nanomagnets, quantum materials

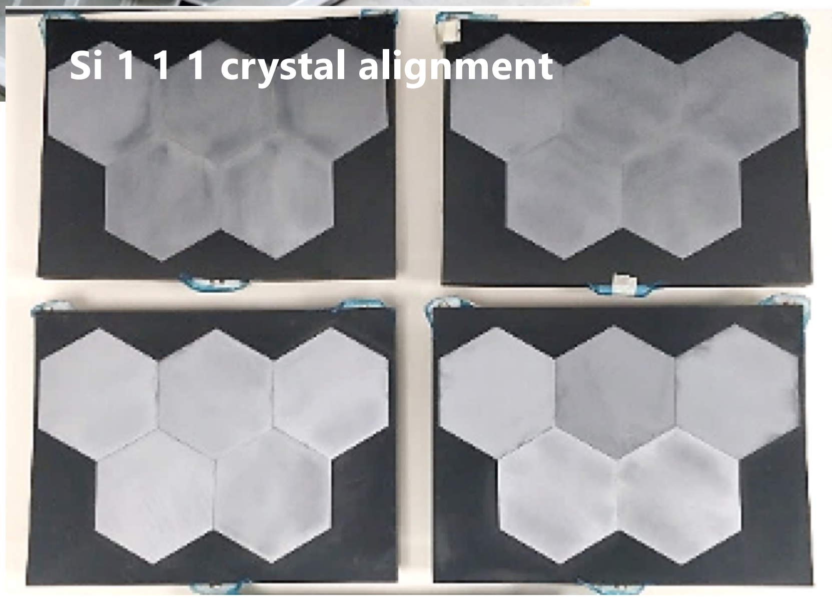
MIRACLES Quick Facts	
Instrument Class	Spectroscopy
Moderator	Cold
Primary Flightpath	162.5 m
Sample-Analyser Flightpath	2.5 m
Wavelength Range	2–20 Å
Bandwidth	1.5 Å, ±0.5 meV[a]
Energy Transfer Range	−2 to +20 meV
Q Range	0.2–2 $Å^{-1}$[a]
High Flux Mode	
Flux at Sample at 2 MW	1.5×10^{9} n s^{-1} cm^{-2}[a]
Elastic Energy Resolution	45 μeV
High Resolution Mode	
Flux at Sample at 2 MW	4×10^{7} n s^{-1} cm^{-2}[a]
Elastic Energy Resolution	2 μeV

[a]When centred on $\lambda = 6.27$ Å.



MIRACLES

Backscattering Spectrometer



Successes

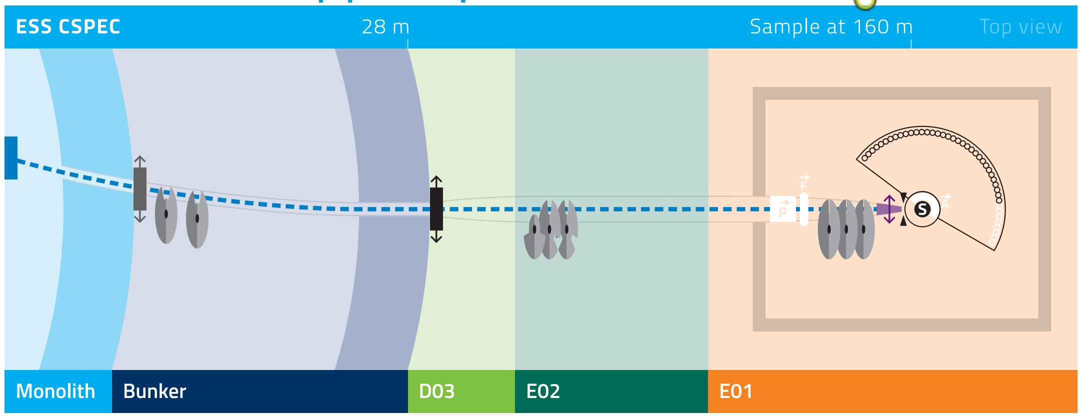
Guides delivered to ESS.
Radial collimator delivered.
Chopper cascade under manufacturing.
Assembly of mechanical parts for choppers initiated.
Successful tests of the Si 111 analyser crystals on IN16b.
Manufacturing of detector tank is progressing.
CAVE and control cabin will shortly be tendered.
Successful tests of detector chain.

Concerns

No MIRACLES staff at ESS.
No progress in common projects (electrical/utilities).
No PE shielding for fast neutrons considered.

CSPEC

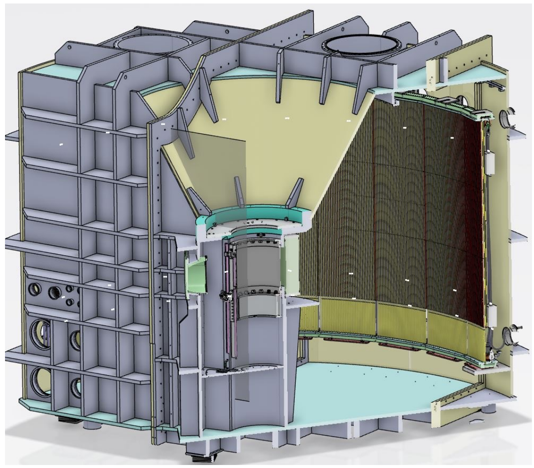
Cold Chopper Spectrometer



- **Quantum materials:** Low lying excitations of quasiparticles in quantum materials.
- **Magnon -phonon hybrid excitations** in multiferroic materials.
- **Enzyme catalysis**: Time dependence of the rotational and translational diffusive processes in enzyme catalysis.
- **Hydration processes:** Dynamics and the structural relaxation of the glassy water.
- **Hydrogen storage:** Time dependent phenomena in clathrates.
- **Metal organic frameworks:** Proton diffusion.
- **Photosynthesis:** Operando studies of proteins.

CSPEC quick facts

Primary flight path	160 m
Secondary flight path	3.5 m
Moderator	Cold
Wavelength range	2-20 Å
Bandwidth	1.72 Å
Flux at sample (2 MW, λ = 5 Å, $\Delta E/E_i$ = 3%, no RRM, with RRM ~ x6)	3×10^6 n s^{-1} cm^{-2} (4 x 2 cm^2 standard beam) 4 10^6 n s^{-1} cm^{-2} (1 x 1 cm^2 focussed beam)
Full detector coverage	-30^o – 140^o [H] ± 26^o [V]
Energy resolution	1.5% - 5% E_i
Polarisation analysis	Foreseen upgrade



CSPEC

Cold Chopper Spectrometer

Successes

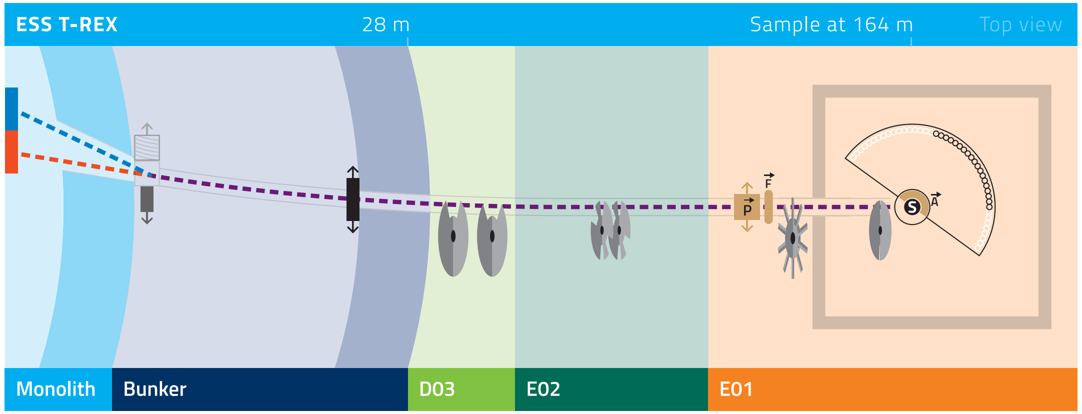
Majority of guides (90%) delivered to ESS.
Radial collimator delivered.
Delivery of 35 T detector tank: July 2024.
CAVE tendered and final design complete.
Chopper manufacturing (accept delays).
Monitor technology agreed upon & being tested.

Concerns

Detector contract (with ILL) still not finalised.
Contract for monitors unclear.
Possible delays due to new ESS quality gate process.
Sample environment not currently prioritised.
Data chain elucidated.

T-REX

Polarised Bispectral Chopper Spectrometer



T-REX Quick Facts	
Instrument Class	Spectroscopy
Secondary Flightpath	3 m
Moderator	Bispectral
Primary Flightpath	164 m
Wavelength Range	0.7–6.5 Å
Bandwidth	1.7 Å
Incident Beam Polarisation	Optional
Polarisation Analysis	Optional
Flux at Sample at 2 MW (E_i = 8 meV)	0.8–5 × 10^6 $ns^{-1}cm^{-2}$
Flux at Sample at 2 MW (E_i = 50 meV)	0.3–2 × 10^6 $ns^{-1}cm^{-2}$
Detector Coverage	1°– 72° [H] × −25°–15° [V] (−36°–144° [H] × −25°–15° [V][a])
Energy Resolution (E_i = 2 meV)	Adjustable 1%–2.5% of E_i
Energy Resolution (E_i = 100 meV)	Adjustable 4%–7% of E_i
[a]) Available as a foreseen upgrade.	

- **Quantum magnetism:** Spin–orbit coupling in the classification of quantum spin liquids
- **Frustrated magnetism**: Crystal field levels of emergent phenomena in magnetically frustrated materials.
- **Energy research:** separation of coherent and incoherent contributions.
- **Gas purification & catalysis:** The role of phonons in MOF's.
- **Metals and Alloys:** Ordering mechanism of solidification
- **Translational and librational vibrations:** structural water molecules.
- **Protein complexes:** Understanding light induced dynamics of antenna pigment/protein complexes.

T-REX

Polarised Bispectral Chopper Spectrometer

Successes

NBOA Guide installation (first component).
Neutron guide manufacturing (SDH).
Detector tank under construction.
Heavy shutter manufactured.
Cold polariser manufactured.
Final design: BL shielding and Cave shielding
Final design: Choppers (Fast & Slow & FAN chopper)
Re-initialise MG detector project.

Still in design:

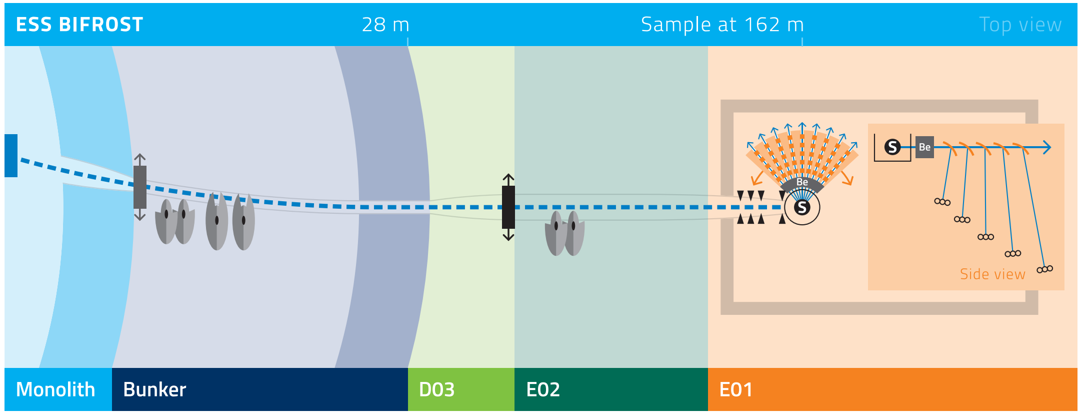
PA equipment
(In-house devices, a lot of work to comply to ESS requirements.)
Primary collimator
Radial oscillating collimator

Concerns

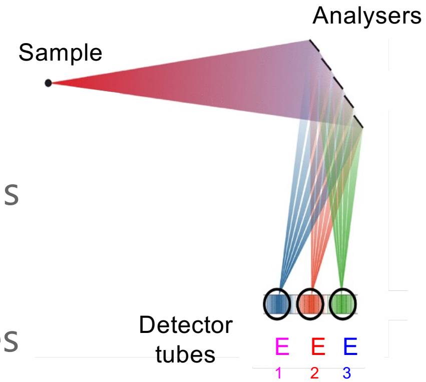
Detector development.
No T-REX staff at ESS.

BIFROST

Multiplexing Indirect Spectrometer for Extreme Environments



- Low-D magnets
- High-Tc superconductivity
- Functional magnetic materials
- Geoscience
- Parametric studies
- Weak signals & small samples

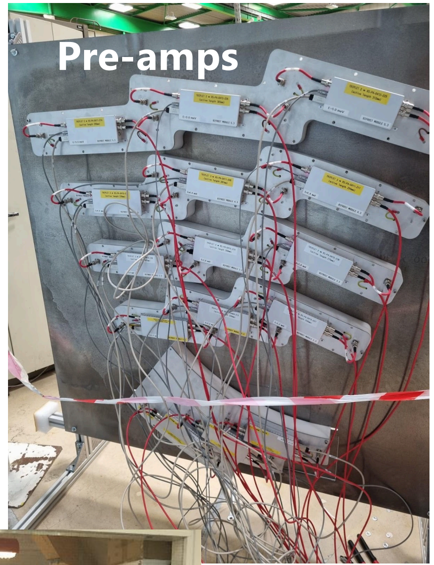


BIFROST Quick Facts.

BIFROST Quick Facts	
Instrument Class	Spectroscopy
Moderator	Cold
Primary Flightpath	162 m
Sample-Analyser Flightpath	1.1–1.7 m
Wavelength Range	1.5–6 Å
Bandwidth	1.7 Å
2θ Range	7°–135°
2θ Coverage	90° in 2 settings
2θ Resolution	0.7°–1.2°
Analyser Energies	2.7, 3.2, 3.8, 4.4, 5.0 meV
Energy Transfer Range	−3 to +55 meV
High Flux Mode [2.3–4.0 Å]	
Flux at Sample at 2 MW	6×10^9 n s^{-1} cm^{-2}
Resolution ($E_f = 5$ meV, $\hbar\omega = 0$)	190 μeV
Resolution ($E_f = 5$ meV, $\hbar\omega = 5$ meV)	450 μeV
High Resolution Mode [2.3–4.0 Å]	
Flux at Sample at 2 MW	9×10^8 n s^{-1} cm^{-2}
Resolution ($E_f = 5$ meV, $\hbar\omega = 0$)	50 μeV (prismatic)
Resolution ($E_f = 5$ meV, $\hbar\omega = 5$ meV)	50 μeV (prismatic)

BIFROST

Multiplexing Indirect Spectrometer for Extreme Environments



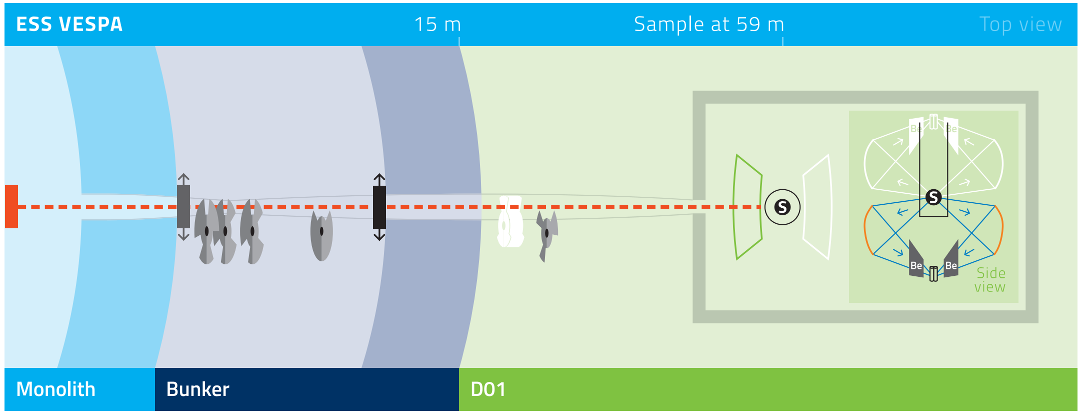
Successes
Detector tank
Guides
Cave/control cabin
Detector tests
Delivery of Beryllium Filter
Choppers: Initial scope PS discs under manufacture
Choppers: Assembly trial fitted in bunker to check interfaces/remote handling …

Concerns
Be Filter: First FAT in summer 2023
- Surface radiation issues – Modified but untested
- Damaged masks - Fixed
- Ambient vacuum leak – Seemingly fixed
- Low temperature leak – Currently unsolved

Detector calibration: Debug in mounted condition, may need cable changes, preamp fixes etc..

VESPA

Vibrational Excitation Spectrometer with Pyrolytic graphite Analysers



VESPA Quick Facts	
Instrument Class	Spectroscopy
Moderator	Thermal
Primary Flightpath	59 m
Sample-Analyser Flightpath	0.61–0.69 m
Wavelength Range	0.4–4.7 Å
Bandwidth	4.3 Å
Analyser Coverage	0.75 (5.25[a]) sr
Analyser Energies	3.7–4.8 meV
Energy Transfer Range	−1 to +500 meV
High Flux Mode	
Flux at Sample at 2 MW	2.3×10^8 n s^{-1} cm^{-2}
Energy Resolution	$\Delta E/\hbar\omega \approx 2.6\%$
High Resolution Mode	
Flux at Sample at 2 MW	6.5×10^7 n s^{-1} cm^{-2}
Energy Resolution	$\Delta E/\hbar\omega \approx 1.0\%$

[a]Available as a foreseen upgrade.

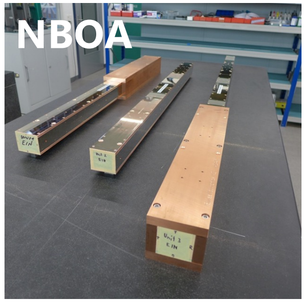
Permit the identification of bonds and functional groups in:

- Solids and liquids.
- soft matter.
- complex fluids.
- bio-materials.

NVS exploits the large incoherent scattering cross section of the hydrogen nucleus. Proton dynamics or vibrations connected to the movement of H atoms can be easily detected spectroscopically, even if hydrogen is dissolved at very low concentrations in materials composed mostly of heavier atoms.

VESPA – VESPA+

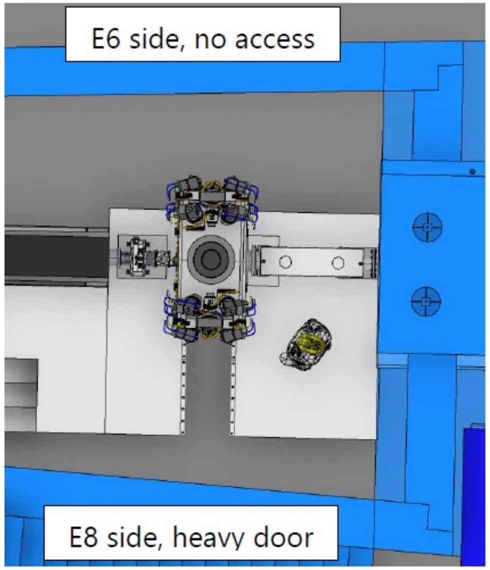
Vibrational Excitation Spectrometer with Pyrolytic graphite Analysers



- Lead instrument scientist (Adrien Perrichon) started at ESS on March 1st
- ESS mechanical engineer position currently advertised
- CNR engineer position signed, to be advertised shortly

REVIEW INSTRUMENT

- Updated McStas model of VESPA primary predicts 25% increase in intensity compared to TG2 baseline
- Frame-overlap single-disk chopper to be replaced by double-disk to better suppress parasitic wavelengths: additional disk can be produced at ESS (extra 175 k€)
- Ongoing review and fine tuning of the chopper positions and slit patterns to optimize flux/resolution
- Proposal to address maintainability and to increase the capacity for sample preparation, sample environments and in situ experiments



VESPA - VESPA+: Rescoping and design modification of the secondary spectrometer are necessary to achieve competitive performance compared to VISION and TOSCA after their upcoming upgrade: VESPA analyzer module design (geometry and spatial arrangement), based on recent progress on TOSCA+, to achieve >7 steradian solid angle coverage

In conclusion

ESS/NSS has developed a great focus to complete the instrument suite.

Project management workload increasing to address complex projects.

No additional resources for solving technical challenges.

Lack of engineering resources across NSS (T2T3 workshops)

ESS needs to take active control of the instruments.

EUROPEAN
SPALLATION
SOURCE

Rescoping (not in order of importance)

(1) Ensure full analyser coverage for MIRACLES.

(2) Full detector coverage for CSPEC

(3) Full detector coverage for T-REX

(4) Upgrade VESPA to VESPA+

In conclusion

ESS/NSS has developed a great focus to complete the instrument suite.

Focus on delivery of milestones.

Project management workload increasing to address complex projects.

No additional resources for solving technical challenges.

Lack of engineering resources across NSS (T2T3 workshops)

ESS needs to take active control of the instruments.