



Neutron Spectroscopy @ ESS

PASCALE DEEN

DIVISION HEAD FOR SPECTROSCOPY
EUROPEAN SPALLATION SOURCE ESS ERIC

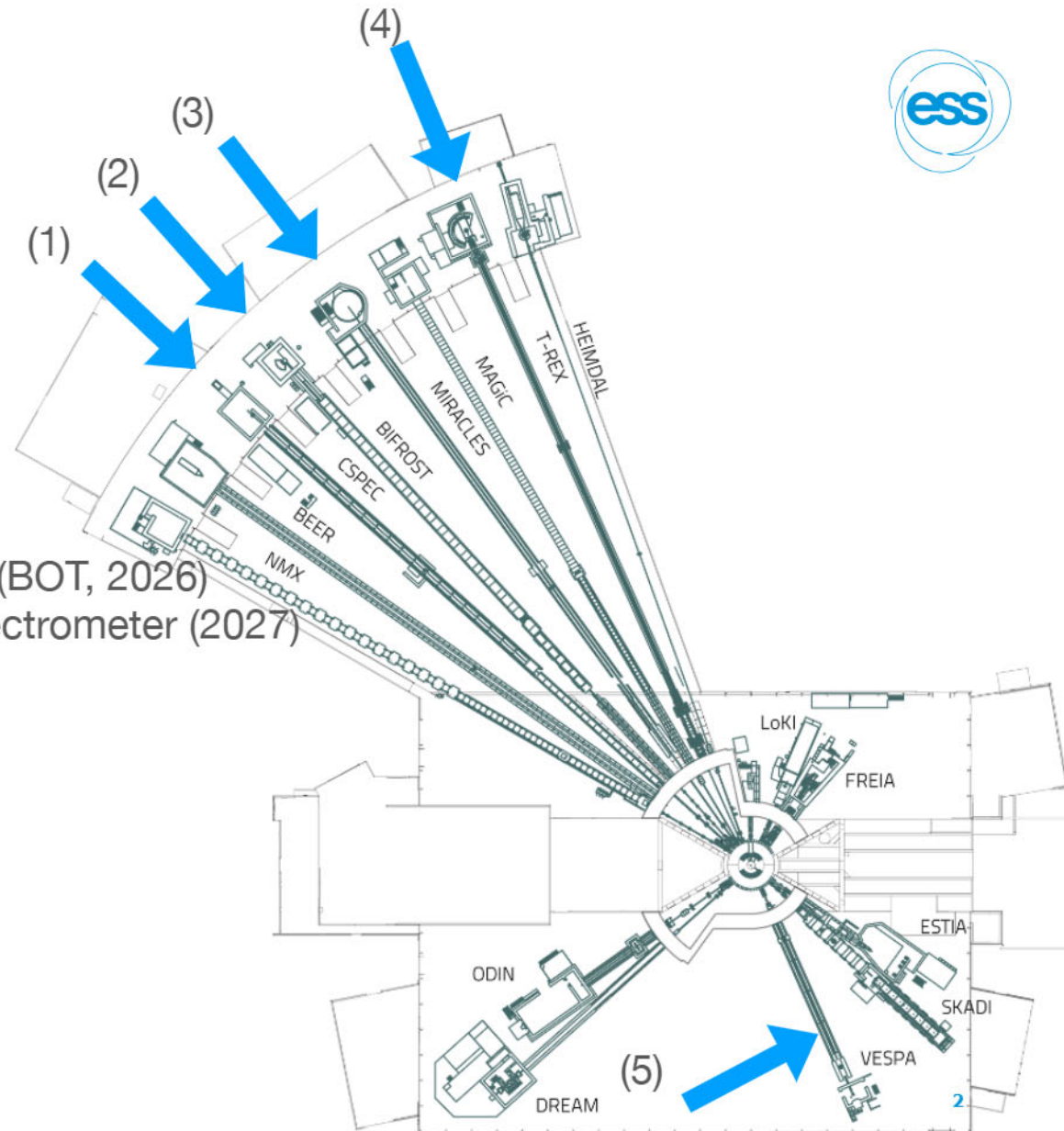
AFFILIATE PROFESSOR: SOLID STATE PHYSICS AND NEUTRON SCATTERING (QUANTUM MAGNETISM)
NIELS BOHR INSTITUTE, UNIVERSITY OF COPENHAGEN

@ ESS SINCE 2011

Spectroscopy division

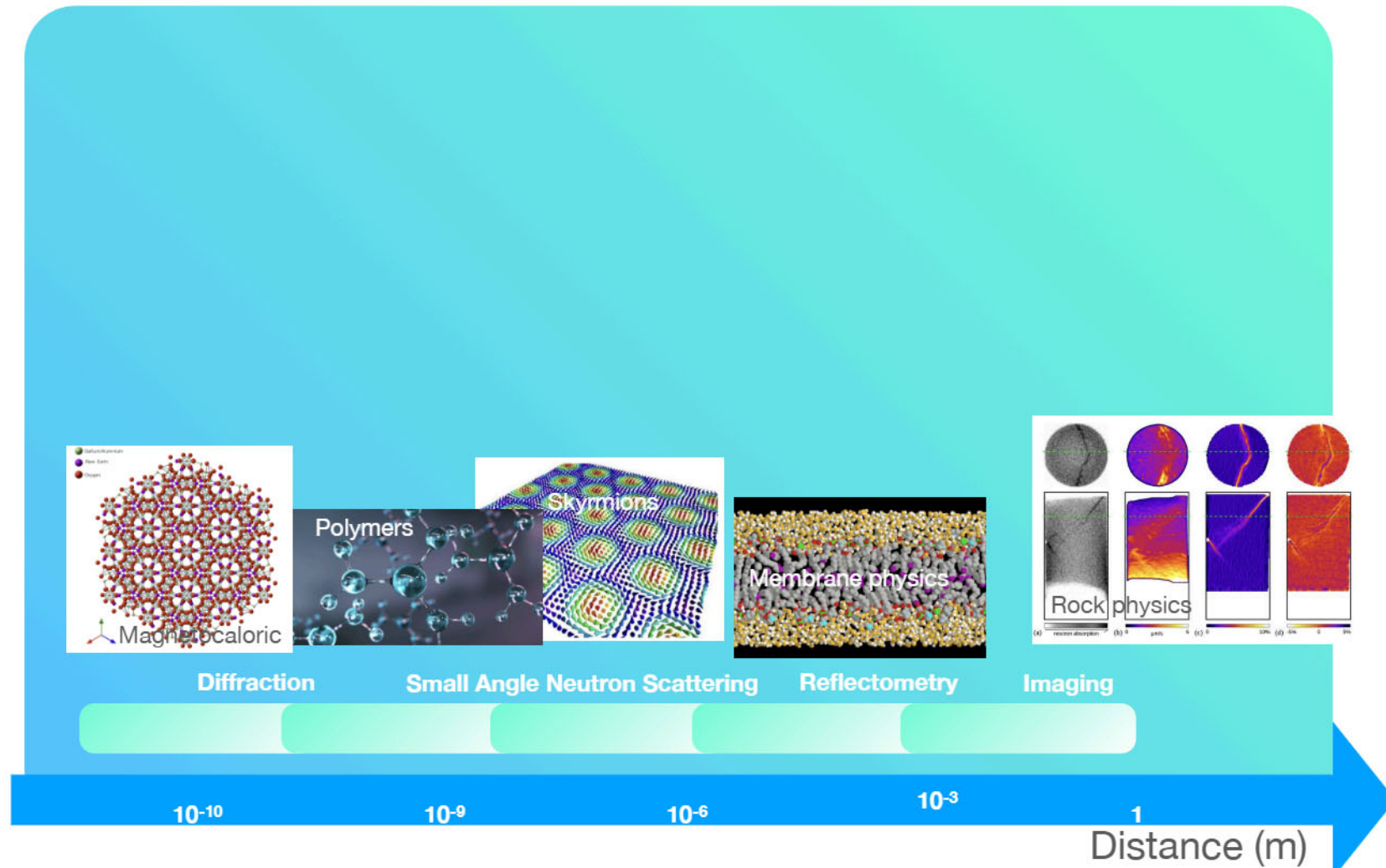


- 1) CSPEC Cold chopper spectrometer (2027)
- 2) BIFROST Extreme Environment Spectrometer (BOT, 2026)
- 3) MIRACLES High resolution Backscattering spectrometer (2027)
- 4) T-REX Bispectral chopper spectrometer (2027)
- 5) VESPA Vibrational Spectrometer (2028)



Spatial and time(energy) scale of materials = functionality

What can neutrons probe



Spatial and time(energy) scale of materials = functionality

What can neutrons probe

Motional dynamics (s)

10^{-14}

Vibrational

10^{-12}

Indirect geometry

Direct geometry

10^{-9}

Backscattering

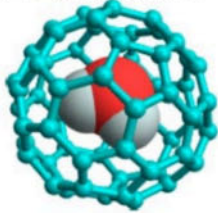
10^{-6}

Spin echo

10^{-3}

1

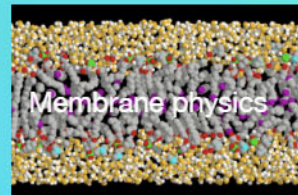
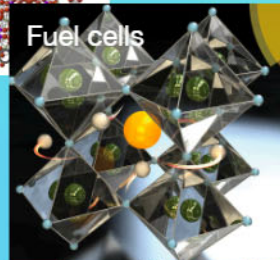
H₂O in fullerenes



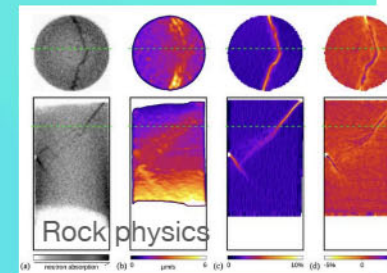
Correlated motions
phonons/magnons



Magnetics



Membrane physics



Distance (m)

Spatial and time(energy) scale of materials = functionality

What can neutrons probe

Motional dynamics (s)

10^{-14}

Vibrational

10^{-12}

Indirect geometry

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10^{-9}

Backscattering

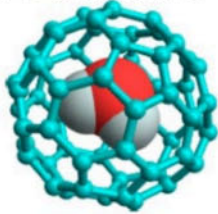
10^{-6}

Spin echo

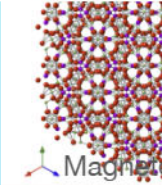
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1

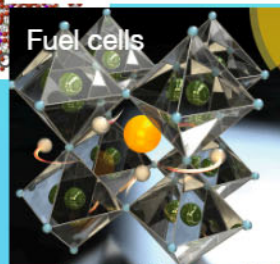
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Correlated motions
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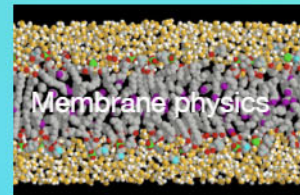
Magnetics



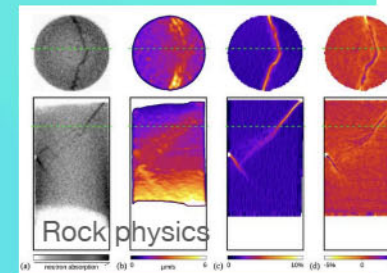
Fuel cells



VESPA
T-REX
BIFROST
CSPEC
MIRACLES



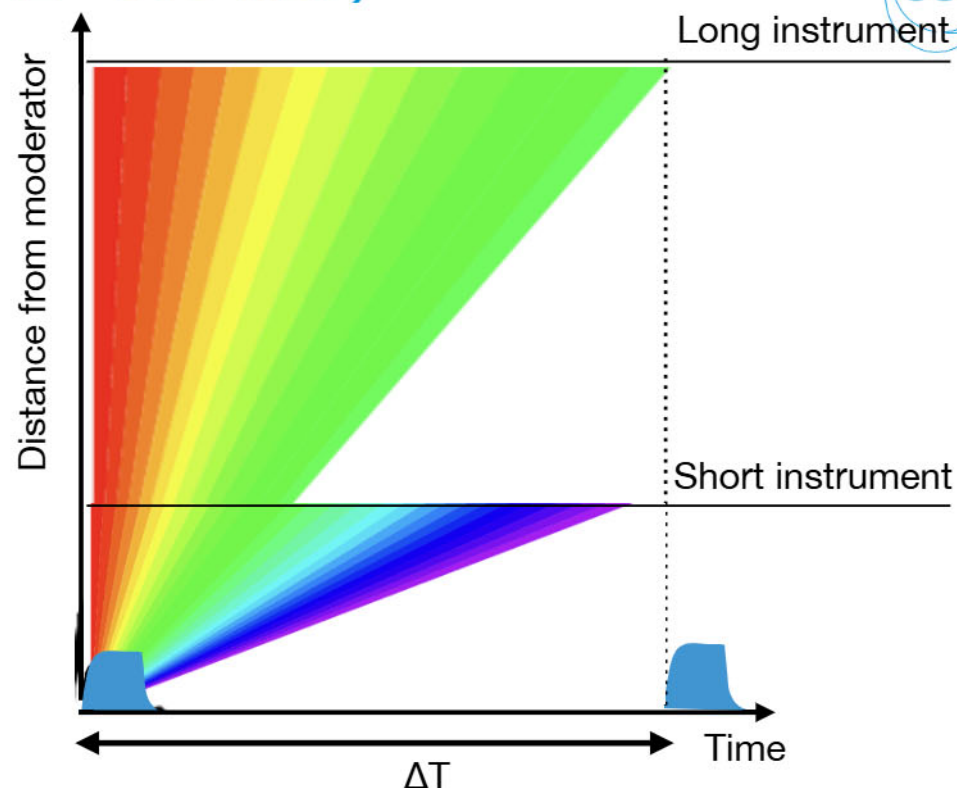
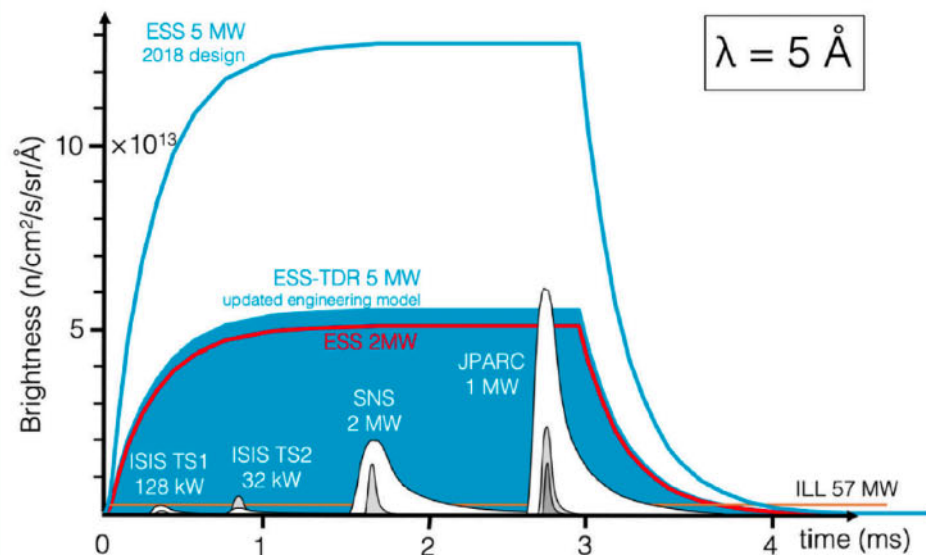
Membrane physics



Distance (m)

European Spallation Source

Long pulse of (mainly) cold neutrons (0.2 - 300 meV)



Long pulse: Spectroscopy: Opportunities from Reactor & Spallation facilities

High signal (long pulse) to noise (spallation)

Wavelength band - broad (short instruments), focussed (long instruments)

$S(\mathbf{Q}, \omega)$: Unparalleled energy resolution nano to meV: trade energy for flux.

Strength of neutrons: $S(\mathbf{Q}, \omega)$ - Born approximation. Optimise work flow from data to understanding (DMSC)

Time dependent phenomena.

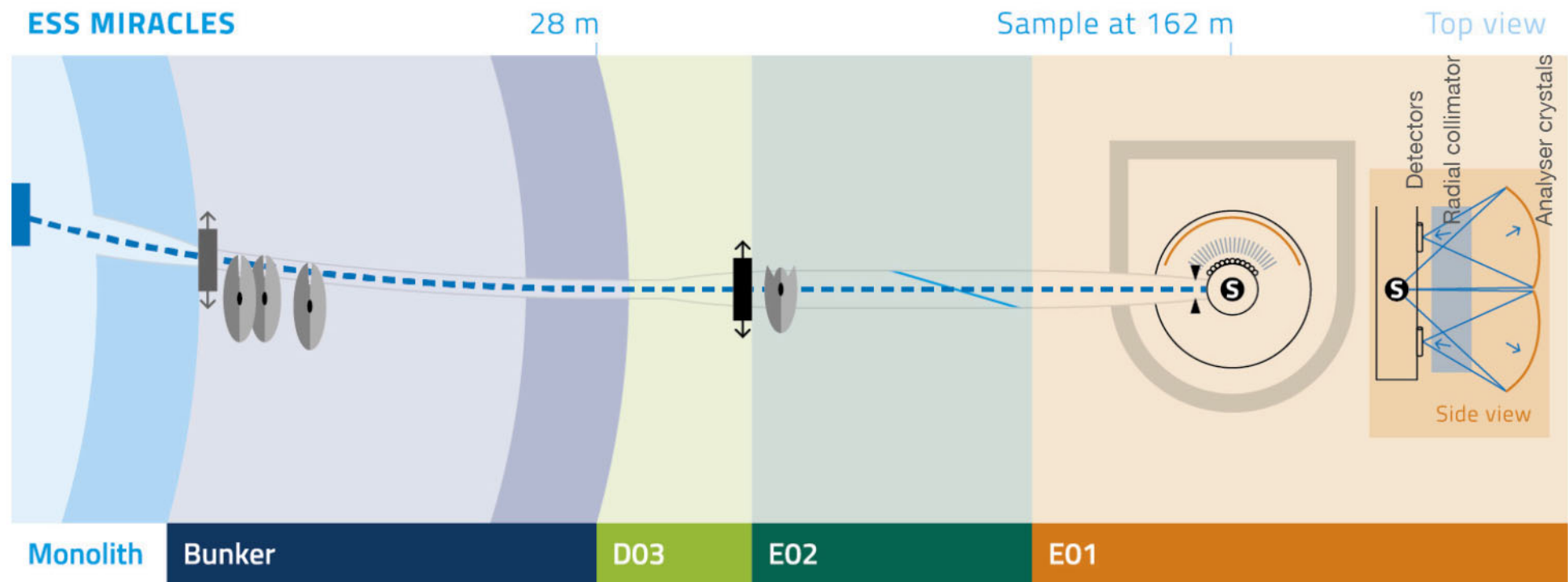
MIRACLES: High resolution backscattering spectrometer



ESS
bilbao



Lead scientist: Felix Villacorta, ESS scientist: Benedetta Rosa, Data scientist: Christian Beck
Lead instrument engineer: Alex Conde Estebanez



Financiado por
la Unión Europea
NextGenerationEU



EUSKO JAURLARITZA
GOBIERNO VASCO

MIRACLES: High resolution backscattering spectrometer

Science case:



Dynamics of proteins and water

Degenerative diseases: Alzheimer, Parkinson, Cancer
Protein dynamics and enzyme catalysis

Drug delivery

Pharmaceutical studies: drug implementation/delivery

Energy sciences:

Proton diffusion in MOFs
Fuel cells and H₂ storage (hydrides)
Catalysis

Polymer sciences:

Viscoelasticity
Morphology-performance connections in e.g. organic electronic devices

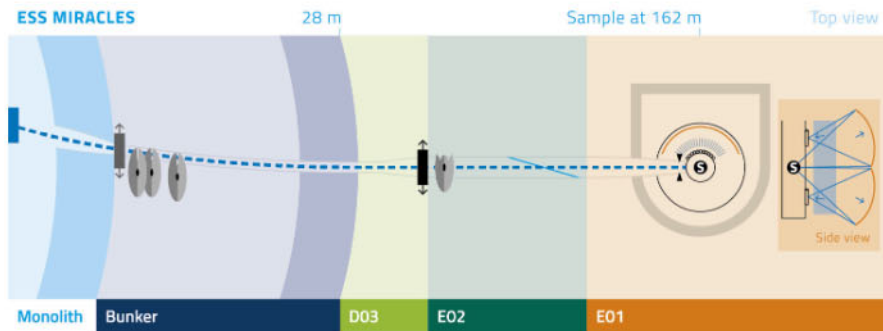
Climate change:

Ice formation
Portland-alternative cements (water dynamics)

Smaller, more dilute or more complex samples

MIRACLES: High resolution backscattering spectrometer

Soft matter, disordered systems, biological matter



- Near backscattering ($2\theta \approx 88.5^\circ$): Si(1 1 1), (3 1 1) & (3 3 3)
- $\delta E = 2\mu\text{eV} - 45\mu\text{eV}$
- Beam spot at sample: $3 \times 3 \text{ cm}^2 - 1 \times 1 \text{ cm}^2$
- Detector coverage = 155° (Hor), $\pm 22^\circ$ (Ver)
- Q range = $0.2 - 2 \text{ \AA}^{-1}$ $\delta Q = 0.2 \text{ \AA}^{-1}$
- ESS timeframe (14 Hz, 71 ms), provides $\pm 500 \mu\text{eV}$
- Radial collimator to provide S/N of 10^4
- Polarisation Analysis

Day 1 sample environments

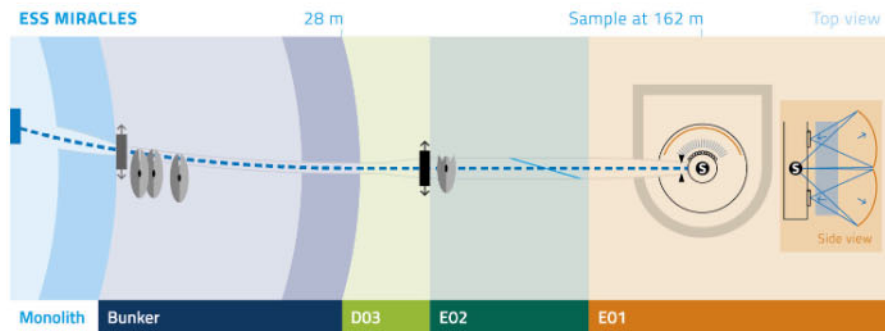
Cryofurnace

Cryostat

Laser pump probe

MIRACLES: High resolution backscattering spectrometer

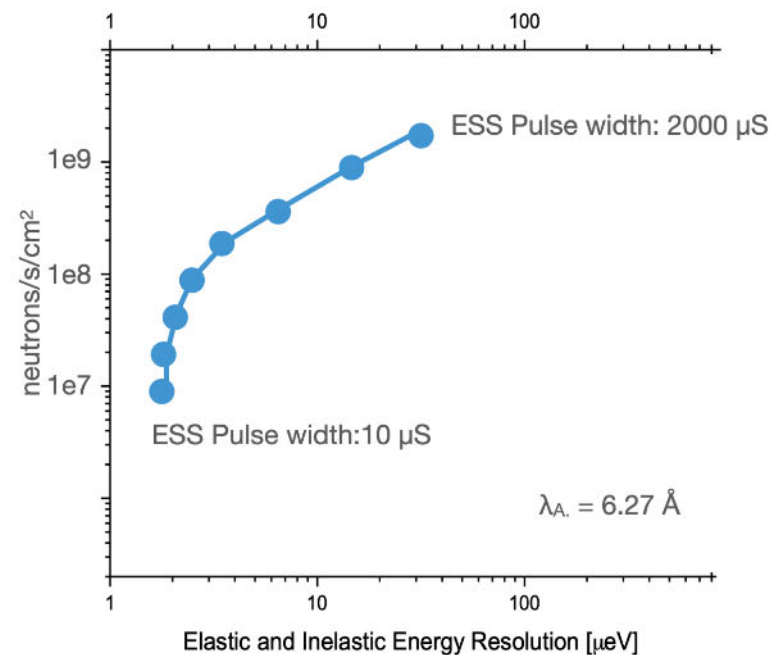
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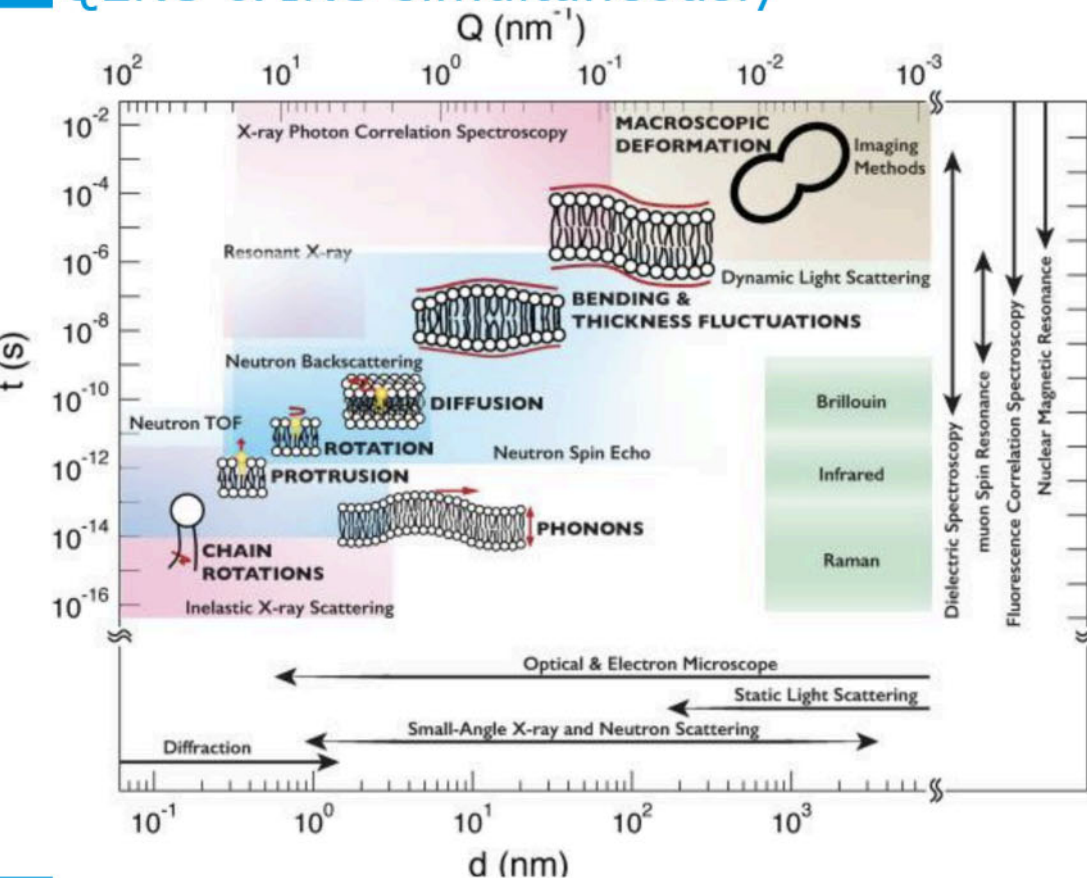
Fluxes and resolution (2 MW)



Flux: 10^7 (2 μeV) - 10^9 (45 μeV) n/s/cm².
Gain of x 9 w.r.t BASIS (SNS) at equal δE .

MIRACLES biologically relevant time-scale (ps-ns)

QENS & INS simultaneously



The temporal and spatial hierarchy of membrane dynamics.

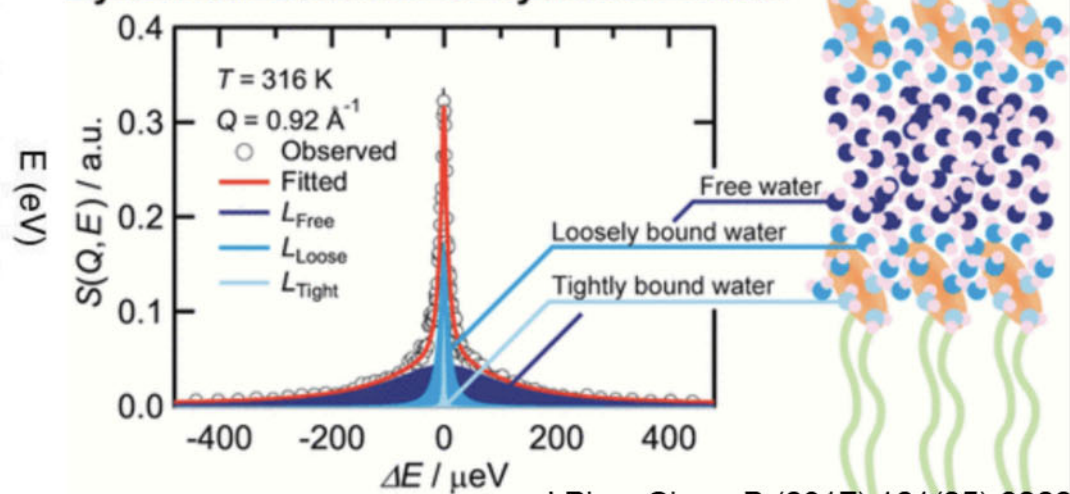
Characterization of Biological Membranes: Structure and Dynamics: Kelley et al.

Data from Pelican/IRIS/IN16B

Fast protein dynamics and stability.



Dynamical Behavior of Hydration Water



J Phys Chem B (2017) 121(35):8322

Study restricted to elastic window scan

QENS = poor statistics.

MIRACLES:

QENS/INS

High flux

Variable energy resolution QENS (flexibility)

Q-dependent measurements

ESS-DEMAX for deuteration

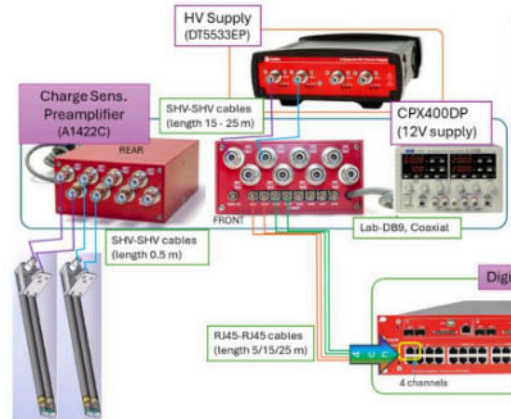
MIRACLES: High resolution backscattering spectrometer

Recent Progress

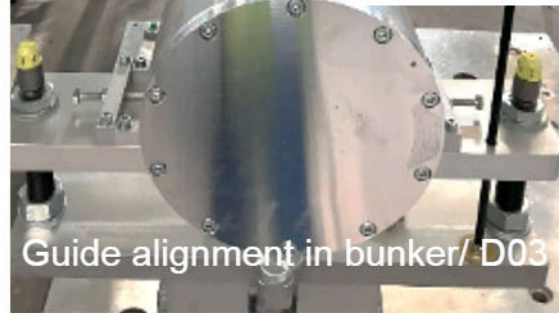
Detector tank delivery to ESS



^3He detectors delivered to ESS



Guide alignment in bunker/ D03



First Science workshop: November 2026

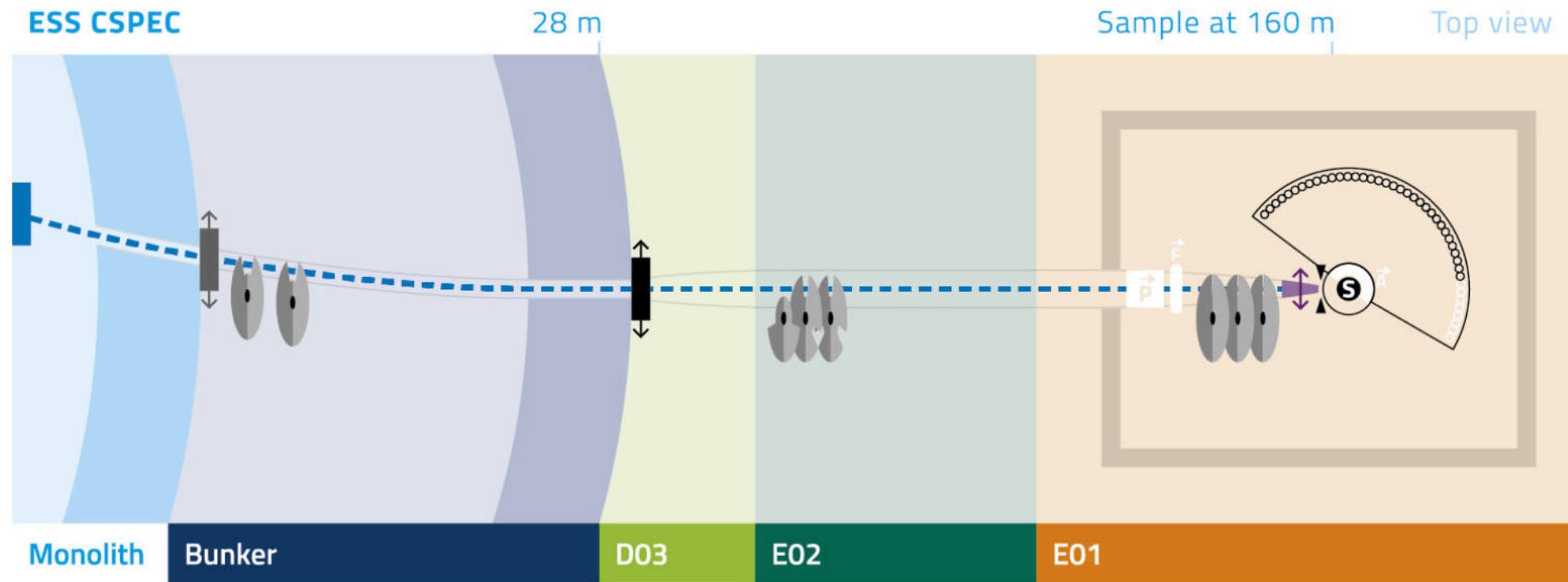


CSPEC: The cold chopper spectrometer of the ESS

Lead scientist: Daria Noferini (functional materials/disorder), [Christian Balz \(magnetism\)](#)

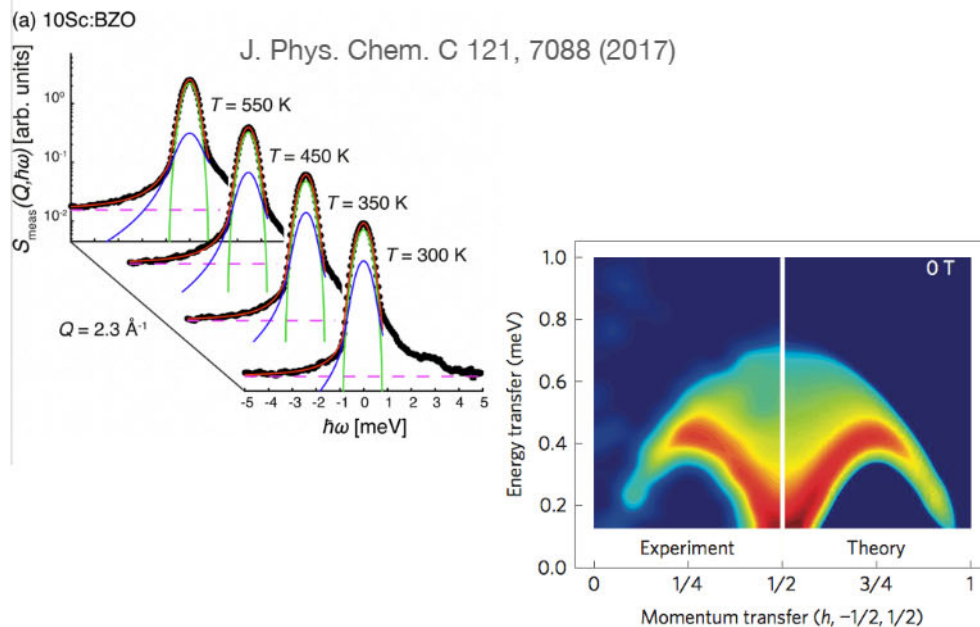
Data scientists: Christian Beck & Greg Tucker

Lead instrument engineer: Fernando Moreira (ESS)



The cold chopper spectrometer of the ESS

Science case:



Nature Physics 9, 435–441 (2013)

Materials: Glass forming, liquid dynamics, crystal growth, hydrogen storage, fuel cells.

Soft matter: Polymer nanocomposites, organic photovoltaics, polymer electrolytes

Biology: protein structure-dynamics-function, cell membrane-protein, drug delivery

Chemistry: ionic liquids, clays, complex fluids

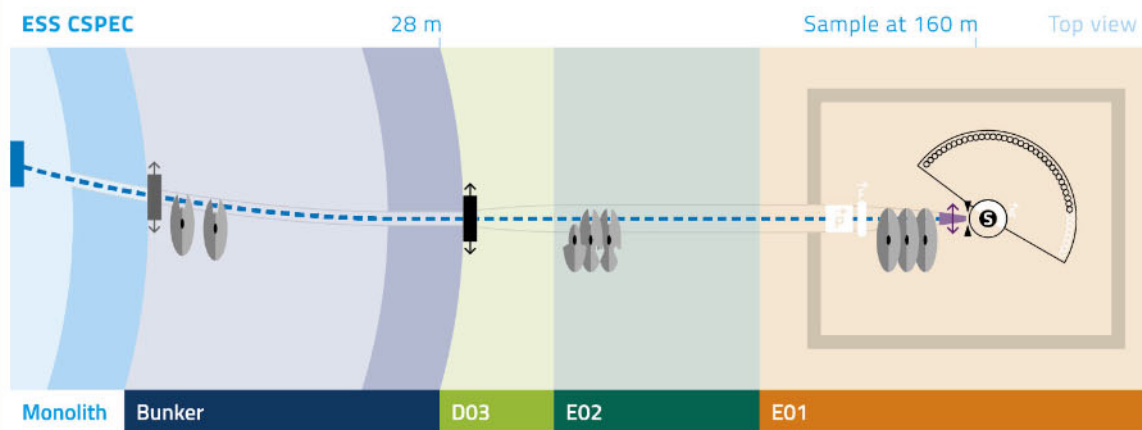
Magnons, phonons, polarons

Topological states of matter: Majorana fermions.

RVB states, Quantum spin liquids, emergent behaviour.

Low lying excitations of materials with a focus on small samples, in-operando/kinetic behaviour
Need 10-50 x current day signal/noise to perform adequately

CSPEC: The cold chopper spectrometer of the ESS

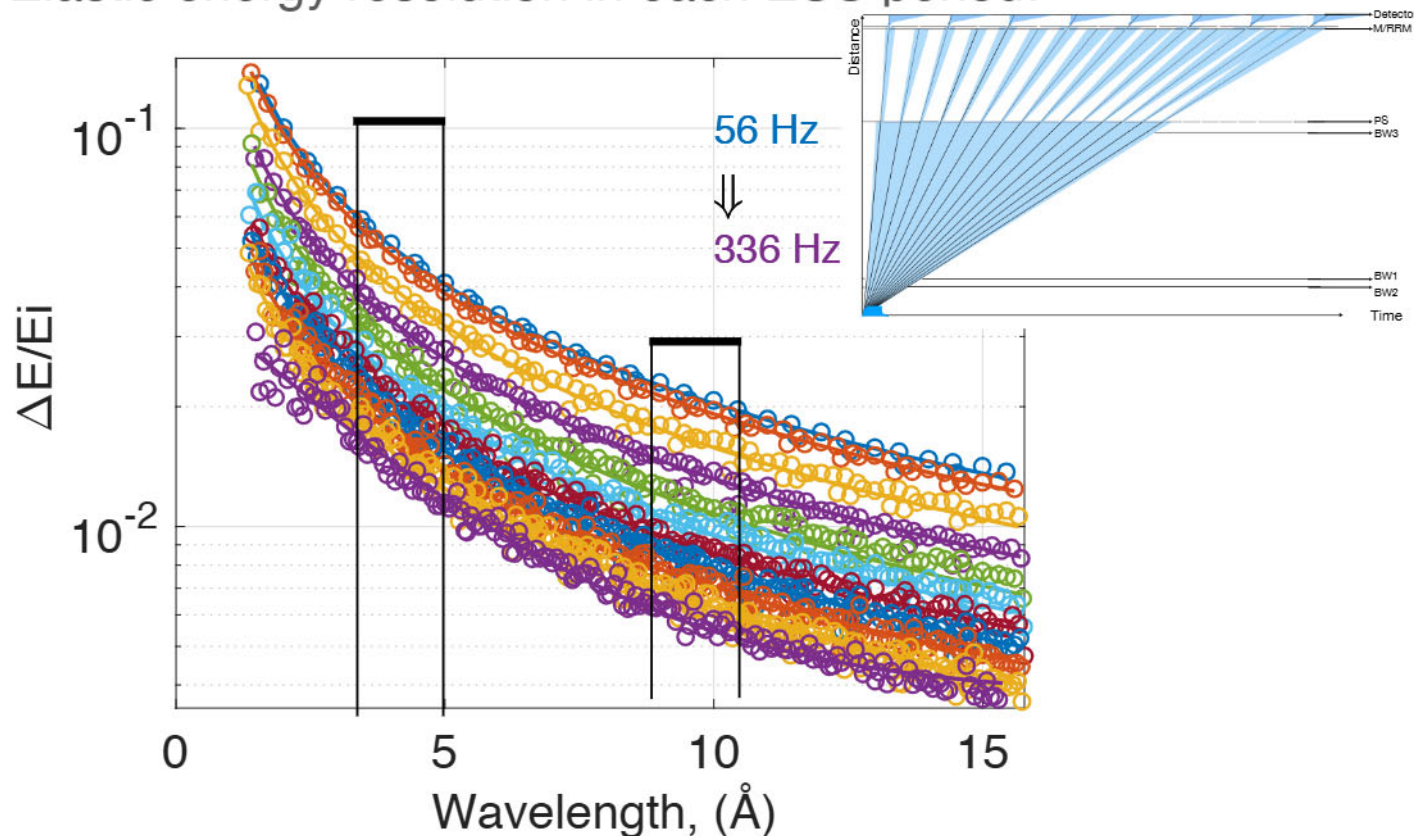


- Moderator to Sample = 160 m
- Cold neutrons (2-20 Å), $\Delta E/E = 1.5\%$ @ 4 Å. FWHM = 80 μeV @ 4 Å
- Focus flux on range of sample areas $4 \times 2 \text{ cm}^2 \rightarrow 1 \times 1 \text{ cm}^2$. FWHM = 6 μeV @ 10 Å
- Signal to noise = 10^5 (@5 Å, Vanadium) - careful collimation & shielding considerations
- Sample to detector: 3.5 m
- Detector coverage $-30 < \theta_H < 140^\circ$, $-26.5 < \theta_V < 26.5^\circ$
- Polarisation analysis (not day 1)

Sample environment: 50 mK - 600 K, 14 T, 2 GPa (hydrostatic & uniaxial)

Primary spectrometer

Elastic energy resolution in each ESS period:



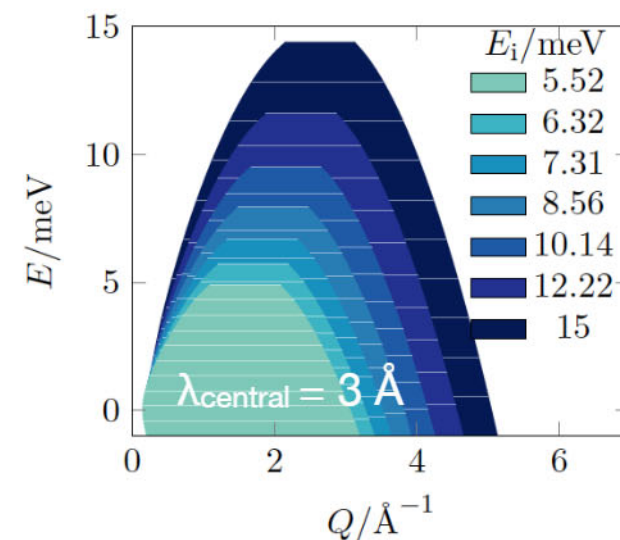
Across accessible bandwidth (1.72 Å)

$$3\text{Å} = 0.023 < \Delta E/E_i < 0.039 \quad (5.52 < E_i < 15 \text{ meV})$$

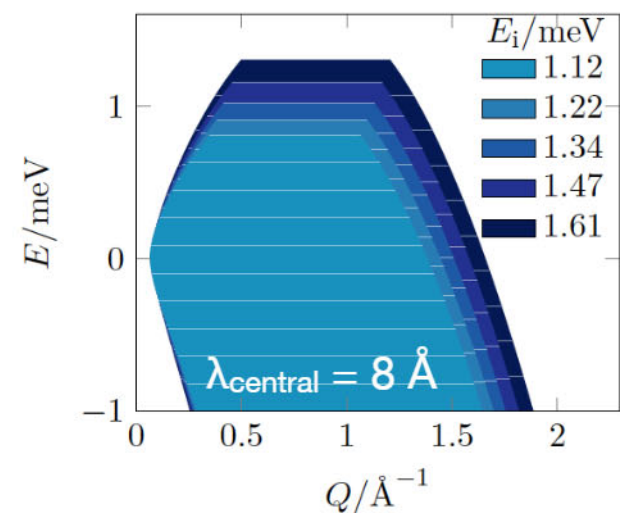
$$8\text{Å} = 0.010 < \Delta E/E_i < 0.012. \quad (1.12 < E_i < 1.61 \text{ meV})$$

Add pulses, gain flux, if possible.

N.B. Single pulse = 4 x IN5: up to 25 x IN5 through effective use of RRM



(b) $5.52 \leq E_i \leq 15 \text{ meV}$



(a) $1.12 \leq E_i \leq 1.61 \text{ meV}$

CSPEC: Understanding proton transport in solid oxides

Rutile TiO₂: A promising anode material for lithium and sodium ion batteries



Giant Enhancement of Hydrogen Transport in Rutile TiO₂ at Low Temperatures

E. J. Spahr¹, L. Wen², M. Stavola², L. A. Boatner³, L. C. Feldman^{4,5}, N. H. Tolk⁵, and G. Lüpke¹

Show more

Phys. Rev. Lett. **104**, 205901 – Published 21 May, 2010

F

Infrared pump probe: Enhances RT proton diffusion by a factor of 9



Enhanced Proton Transport in Nb-Doped Rutile TiO₂: A Highly Useful Class of Proton-Conducting Mixed Ionic Electronic Conductors

Takuma Shiraiwa, Tomoyuki Yamasaki,* Kizuku Kushimoto, Junya Kano, and Takahisa Omata*

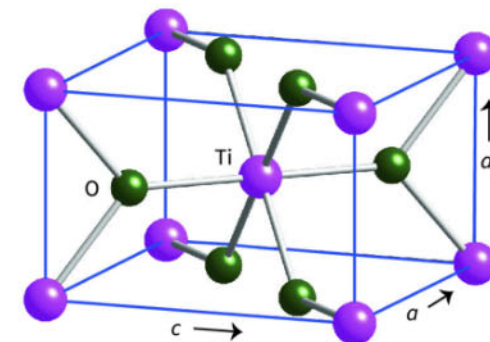


Cite This: *J. Am. Chem. Soc.* 2025, 147, 30757–30767



Read Online

Doping rutile TiO₂ with niobium (Nb) improves proton conductivity and diffusion in the doped material are 10–100× (or more) higher than in undoped TiO₂.

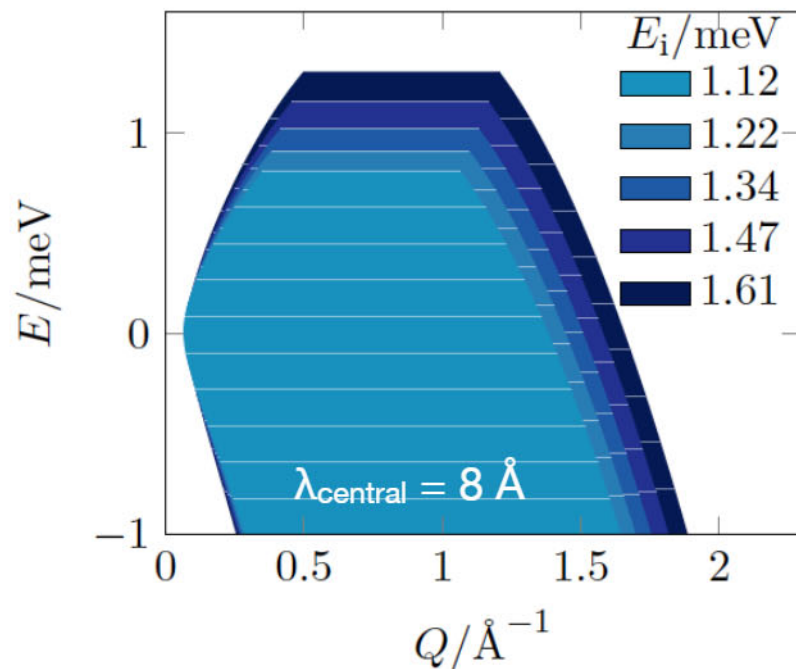


Provides a novel design guideline for mixed protonic and electronic conductors, paving the way for the development of future materials in hydrogen-related electrochemical applications.

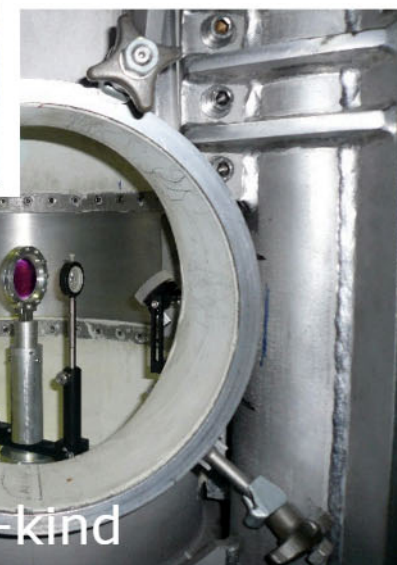
CSPEC: The cold chopper spectrometer of the ESS

Novel scientific opportunities

Opportunities for routine pump
probe spectroscopy



(a) $1.12 \leq E_i \leq 1.61 \text{ meV}$



Estonian in-kind

Wide dynamics and spatial range

Novel use of RRM: Unprecedented flux

Optical enhancement of hydrogen motions: pump probe set-up.

CSPEC: The cold chopper spectrometer of the ESS

Novel scientific opportunities (Polarisation analysis)



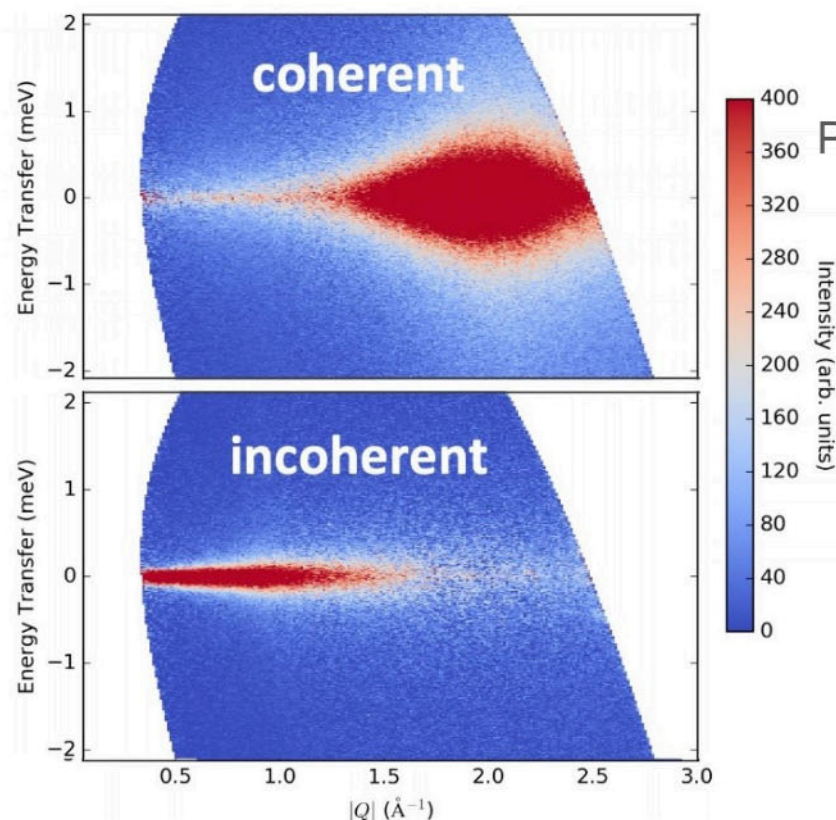
PHYSICAL REVIEW RESEARCH 2, 022015(R) (2020)

Rapid Communications

D₂O

Coherent structural relaxation of water from meso- to intermolecular scales measured using neutron spectroscopy with polarization analysis

Arantxa Arbe¹, Gørn J. Nilsen², J. Ross Stewart², Fernando Alvarez^{1,3},
Victoria García Sakai² and Juan Colmenero^{1,3,4,*}



Generally assumed that replacing D by H is fine
With H - mainly incoherent

With D - mainly coherent : is this the case?

Pair correlations at high Q (intermolecular scales) structural relaxation dominated by diffusion

Self correlations important at low Q (meso scales)

This work opens a way of approaching the unknown territory of coherent scattering from meso to intermolecular scales in

- **Water**
- **H-bonded liquids**
- **Glass forming liquids**
- **Biological systems.**
- **Hydrogen motions in anode materials**

CSPEC: Cold Chopper Spectrometer of ESS



Detector tank in its final place
Precision (+/- 1mm)



Installation of BW choppers in bunker.
All choppers tested and accepted



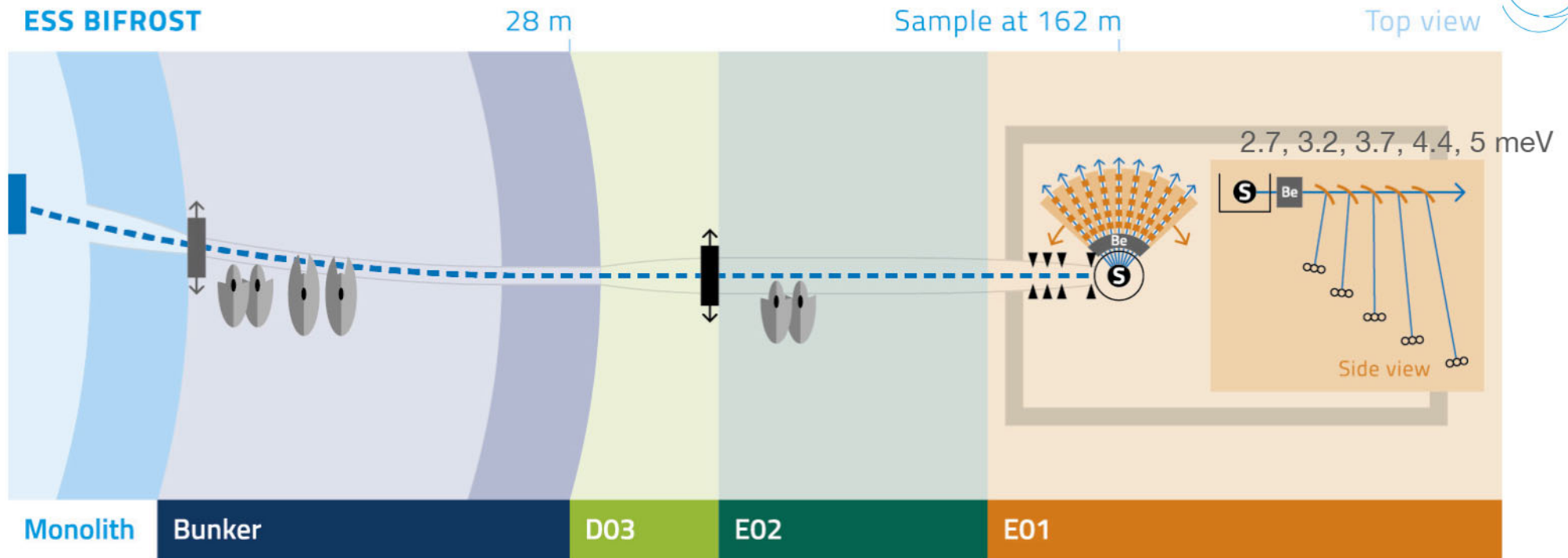
Completion of cave and crane
installation



First Science workshop: Autumn 2026

BIFROST: Triple axis spectrometer for extreme environments

Lead scientist: Rasmus Toft-Petersen, Second scientist, Instrument data scientist: Greg Tucker



PAUL SCHERRER INSTITUT
PSI



DTU Technical
University of
Denmark



IFE Institute for Energy Technology

EPFL
ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

BIFROST: Triple axis spectrometer for extreme environments

Science case:

Quantum magnets / quantum materials / low-dimensional magnets

Unconventional superconductors and strongly correlated electron systems

Functional and multiferroic materials — phase transitions, complex orderings

Energy materials

Efficient screening and discovery of new materials

Evolution towards:

- More complex phenomena:

- fractional excitations
- Line broadening
- Magnon-phonon coupling
- Complex systems

- Smaller samples

- More complex sample environment

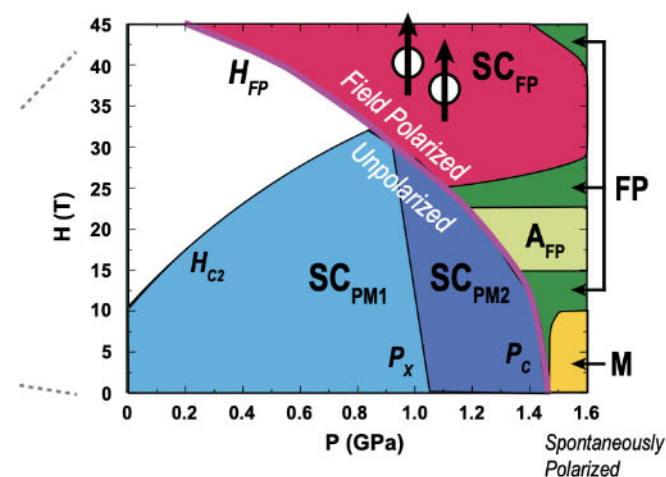


ARTICLE OPEN

[Check for updates](#)

Expansion of the high field-boosted superconductivity in UTe_2 under pressure

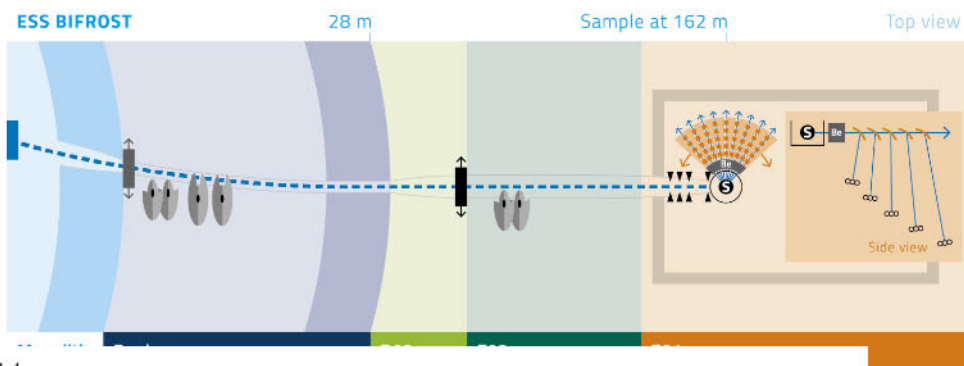
Sheng Ran^{1,2,3}, Shanta R. Saha^{1,2}, I-Lin Liu^{1,2}, David Graf⁴, Johnpierre Paglione^{1,2} and Nicholas P. Butch^{1,2}



Magnet induced Spin-triplet superconductivity

Multiplexing analysers together with the prismatic analyser concept

BIFROST is optimized for **small samples**, and for experiments under **extreme sample environments** (very low temperatures, high magnetic fields, high pressures).



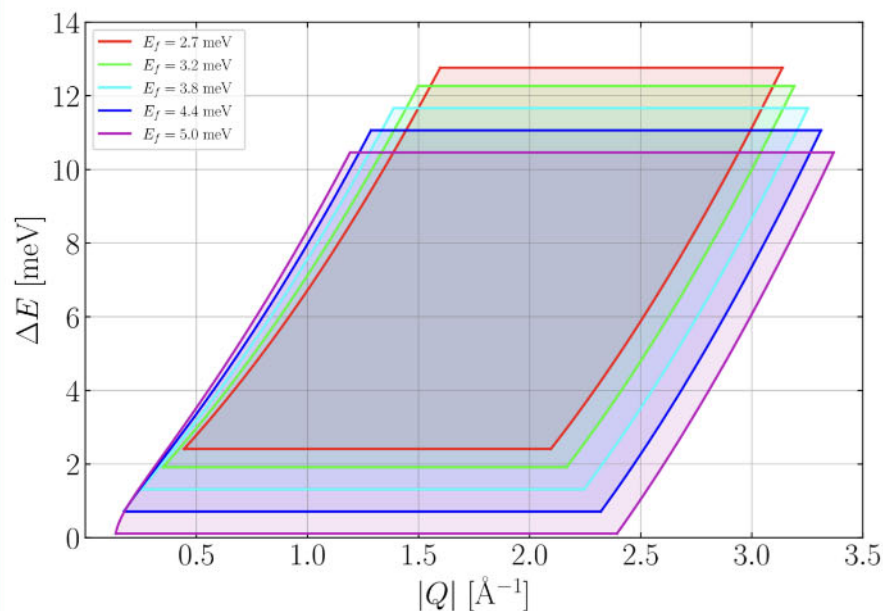
Focus on cold moderator

1.5-6 Å, Bandwidth = 1.7 Å

Sample = 1 x 1 cm² - 0.1 x 0.1 cm²

Indirect Geometry: PG analysers (x 5)

Horizontal 7 - 135°, Vertical angular coverage = ±1.4°



High flux mode : 2 MW (2.3 - 4 Å)
190 μeV (dE = 0.0) = 6e9 n/s/cm²

High resolution mode (2.3 - 4 Å)
50 μeV (dE = 0.0) = 9e8 n/s/cm²

Sample environment: 50 mK - 600 K, 15 T, 2 GPa (hydrostatic & uniaxial)

Topological states of matter: qubits.

Majorana fermions (new state of matter: fundamental and quasi.)

Many-body quantum phase of matter: long-range (topological or quantum) entanglement

Ettore Majorana (1937)

Majorana fermions: particle = antiparticles

Topologically protected.

Resistant to environmental noise (braiding: **changes the quantum state** in a way that depends on the *order* of the exchanges.) .

Noise resistance quantum computing



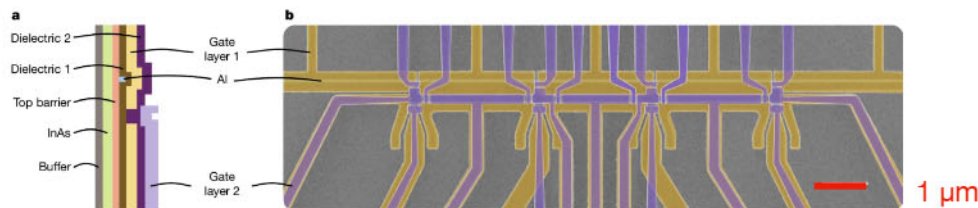
Condensed matter (1) Majorana fermions (electronic states)

In/Ar/Al(SC) hybrid nanowire structures: Quasiparticle excitation - zero edge modes

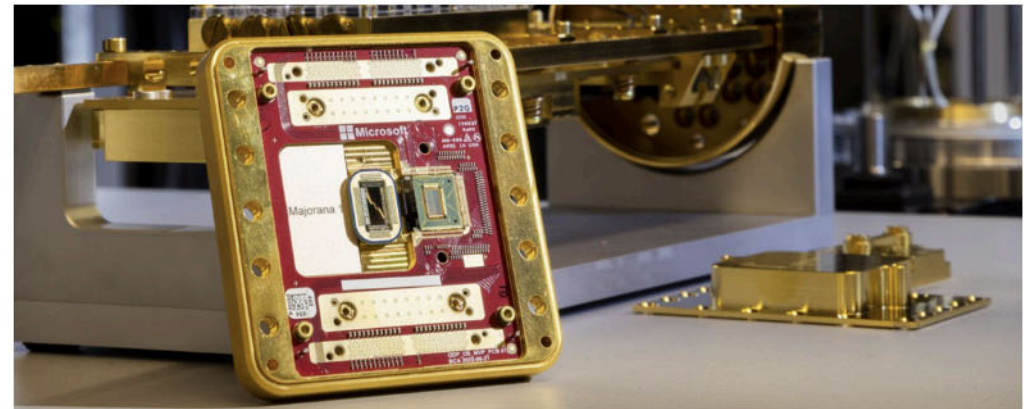
Interferometric single-shot parity measurement in InAs–Al hybrid devices

[Microsoft Azure Quantum](#), [Morteza Aghaee](#), [Alejandro Alcaraz Ramirez](#), [Zulfi Alam](#), [Rizwan Ali](#), [Mariusz](#)

[Nature](#) **638**, 651–655 (2025)



a, Cross-section of the gate-defined superconducting nanowire device design. **b**, Scanning electron microscopy image with the aluminium strip (blue), first gate layer (yellow) and second gate layer (purple) indicated in false colour. Scale bar, 1 μm.



Introducing Microsoft Majorana 1

Scientific opportunities: Topological states of matter: qubits. Majorana fermions (derived from magnetic spins)

Kiteav quantum systems (Bond frustration):

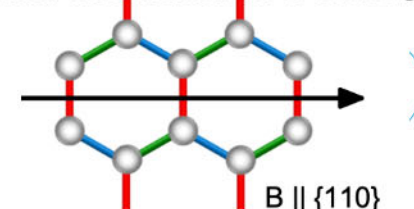
Majorana fermions: entangled magnetic quantum state with topological ordering and fractionalized spin excitations:

$\alpha\text{-RuCl}_3$ has a 2D layered honeycomb structure ($4d^5 \text{Ru}^{3+}$), similar to graphite.

The layers are weakly bound by van der Waals forces $\Rightarrow$ graphene

Signature: Fractionalized spin excitation (from entangled spins) : neutron scattering

Bond frustration in $\alpha\text{-RuCl}_3$

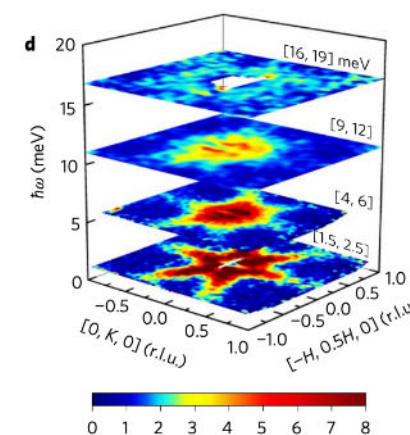
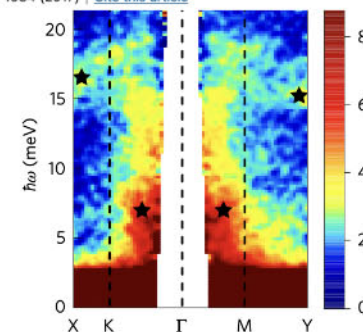


Letter | Published: 18 September 2017

Majorana fermions in the Kitaev quantum spin system $\alpha\text{-RuCl}_3$

Seung-Hwan Do, Sang-Youn Park, Junki Yoshitake, Joji Nasu, Yukitoshi Motome, Yong Seung Kwon, D. T. Adroja, D. J. Voneshen, Kyoo Kim, T.-H. Jang, J.-H. Park, Kwang-Yong Choi & Sungdae Ji

Nature Physics **13**, 1079–1084 (2017) | [Cite this article](#)



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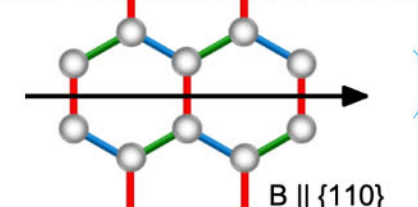
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Signature: Fractionalized spin excitation (from entangled spins) : neutron scattering

Phonons scattered by Majorana fermions in Kiteav QSL.

Sound attenuation to determine new phases

Bond frustration in $\alpha\text{-RuCl}_3$

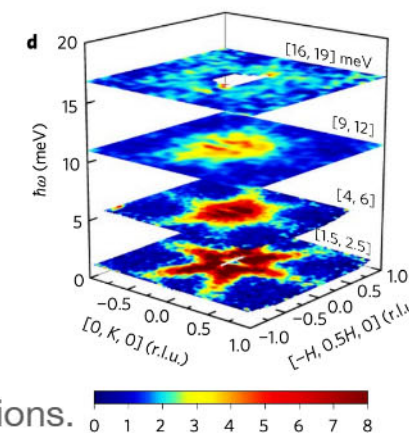
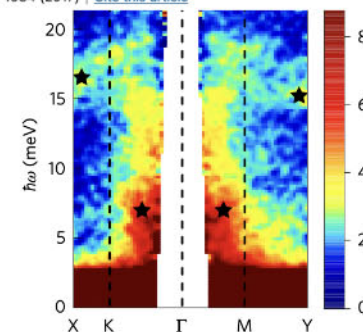


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Nature Physics **13**, 1079–1084 (2017) | [Cite this article](#)



SPIN-STRAIN INTERACTIONS UNDER HYDROSTATIC ...

PHYSICAL REVIEW B **112**, 134405 (2025)

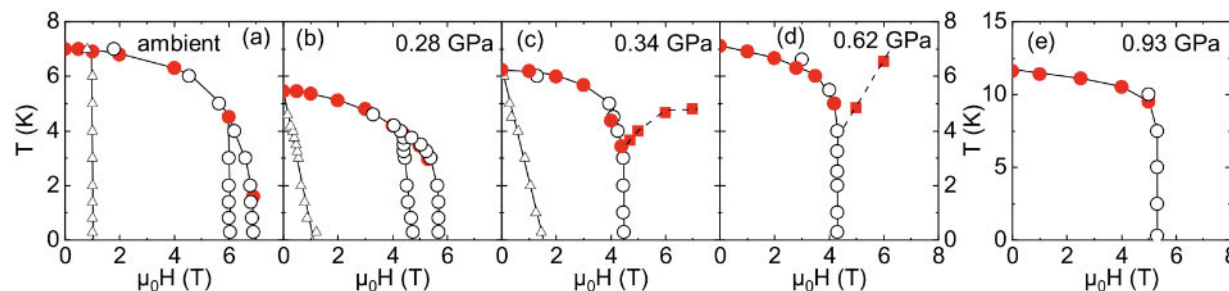


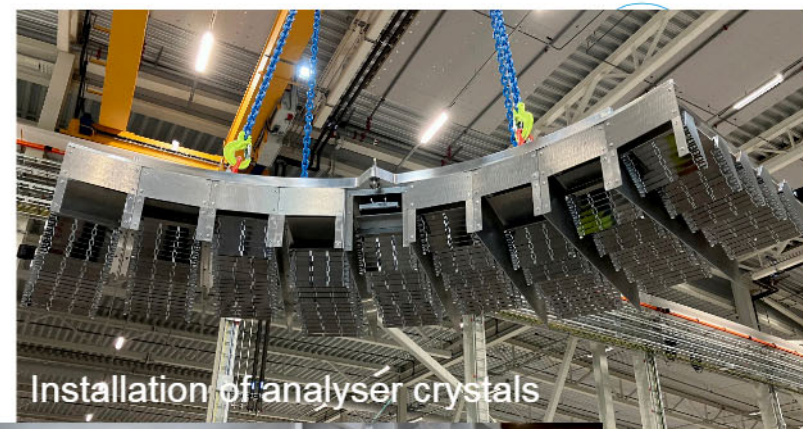
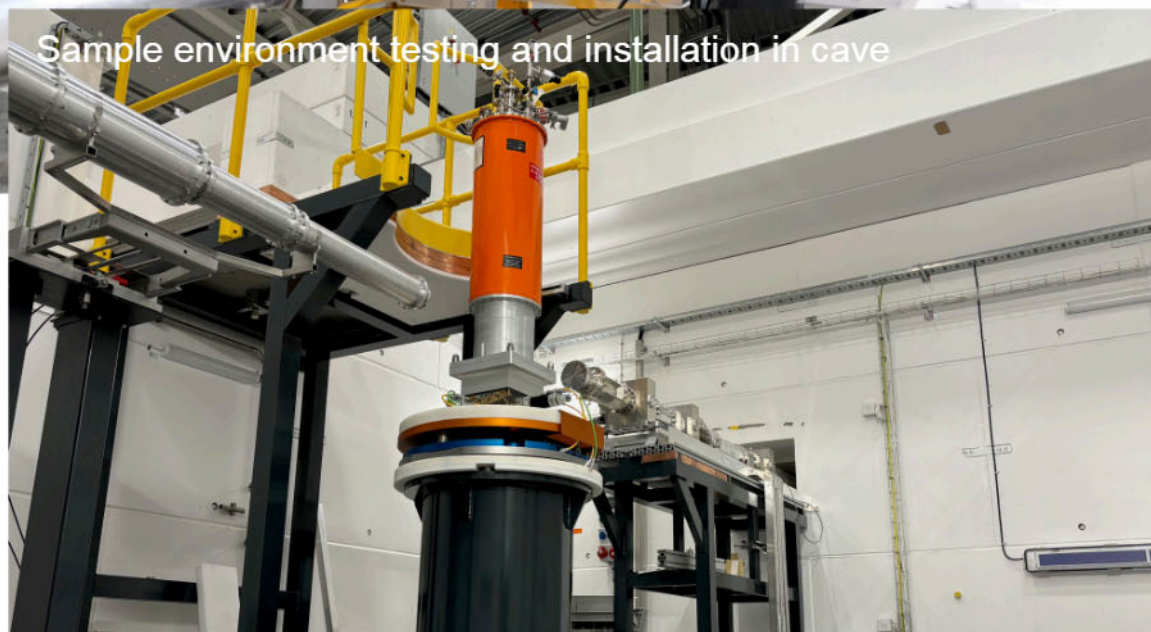
FIG. 5. (a)–(e) H - T phase diagrams ($H \parallel a$) of $\alpha\text{-RuCl}_3$ at various hydrostatic pressures. We extracted critical temperatures from temperature-dependent measurements (red circles) and critical fields from field-dependent measurements (open circles and triangles) from our ultrasound results shown in Figs. 2(a) and 2(b). No transitions have been observed at 1.16 GPa. See text for details.

Pressure reveals an intricate interplay between stacking order, spin gaps, and magnetic transitions.

BIFROST: Extreme environment spectrometer Completed and ready for Beam on Target



Sample environment testing and installation in cave



Installation of analyser crystals

Detector testing and read out chain



Fitting of beryllium filters.

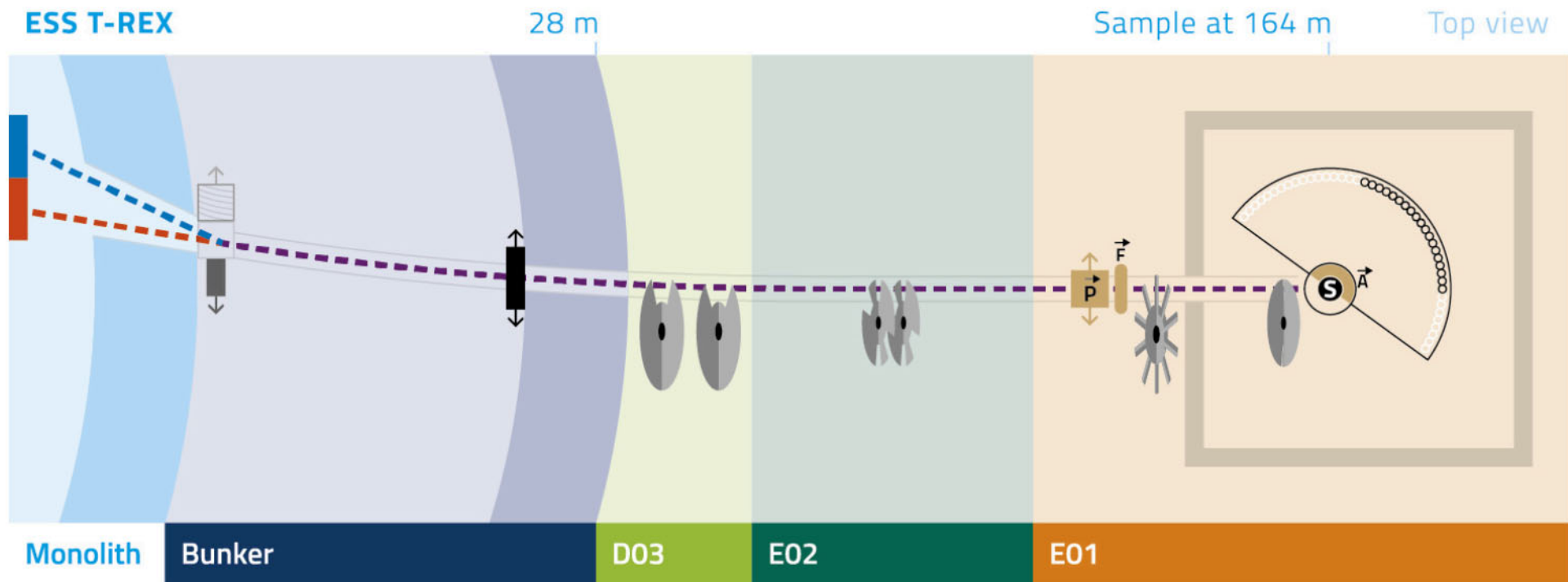
T-REX: Bispectral chopper spectrometer with PA

Lead scientist: Christian Franz,

Scientists: Mohamed Aouane (ESS), Andrea Orechini (Univ.Perugia)

Data Scientist: Bing Li

Lead instrument engineer: Marcel Serwe



T-REX: Bispectral chopper spectrometer with PA

Science case:

Thermoelectrics

A good understanding of thermal conductivity requires knowledge about the phonon density of states

- **Magnons for applications in devices**

Understanding of magnon modes throughout the entire Brillouin zone as a prerequisite for functional applications

- **Itinerant ferromagnetism**

Spin-carrying electrons act as (almost) single particles, requiring large momentum transfers

- **Topological excitations:**

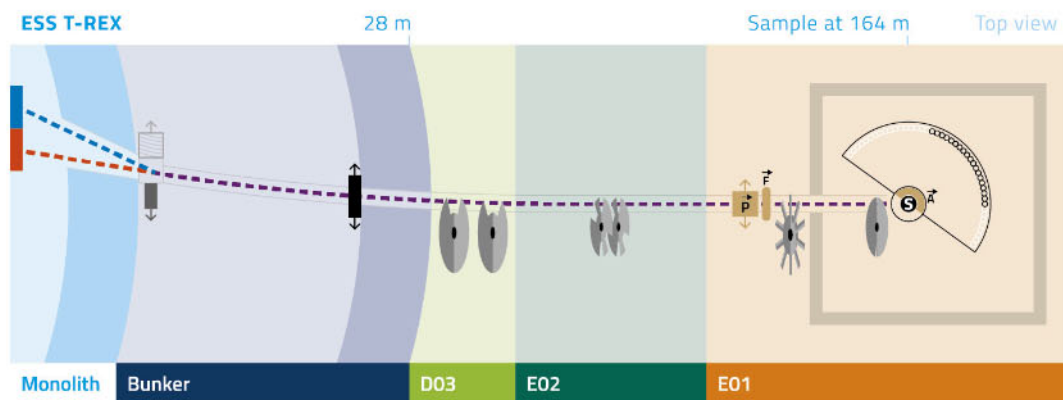
Novel states of matter

- **Hydrogen storage:**

Phonon density of state and self diffusion

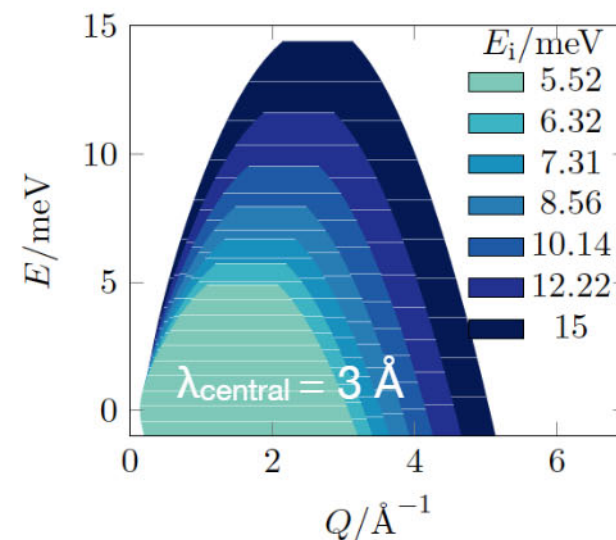


T-REX: Bispectral chopper spectrometer with PA



Moderator to sample = 160 m

- Bi-spectral extraction (0.7-5 Å, 3.5 - 160 meV), $\Delta E/E = 1\% - 7\%$.
- Focus flux on sample area $3 \times 1 \text{ cm}^2$, with optimised divergence
- Sample to detector: 3 m.
- Detector coverage $-30 < \theta_H < 130^\circ$, $-15 < \theta_V < 25^\circ$
- Signal to noise = 10^5
- Polarisation using PASTIS XYZ set-up (Day 1)



(b) $5.52 \leq E_i \leq 15 \text{ meV}$

Broad bandwidth
Many independent pulses.

Sample environment: 50 mK - 600 K, 14 T, 2 GPa (hydrostatic & uniaxial)

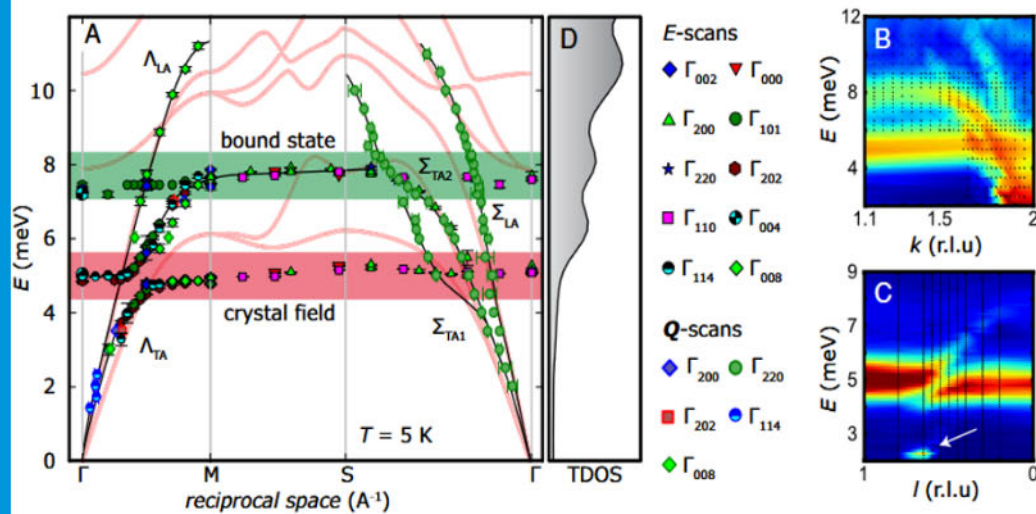
XYZ PA analysis:

Separate the nuclear and magnetic contributions

Magnetoelastic hybrid excitations in CeAuAl_3

Petr Čermák^{a,b,1}, Astrid Schneidewind^b, Benqiong Liu^c, Michael Marek Koza^d, Christian Franz^{e,f}, Rudolf Schönmann^f, Oleg Sobolev^g, and Christian Pfleiderer^{f,1}

Access Kondo physics: basis for many sensors that convert mechanical stress into a magnetic signal



Disentangle optical phonons from a crystal field levels

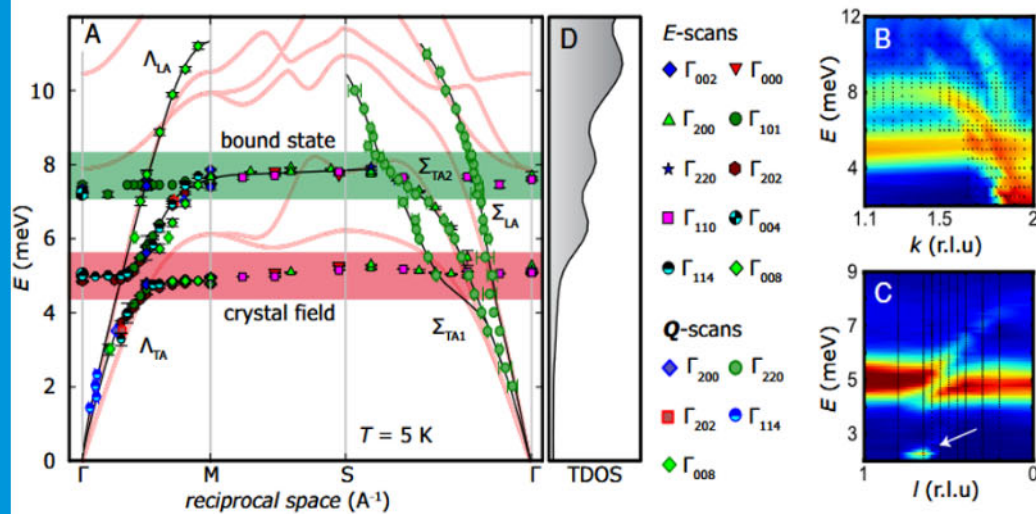
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Access Kondo physics: basis for many sensors that convert mechanical stress into a magnetic signal



Disentangle optical phonons from a crystal field levels

Bispectral extraction (multi E_i mode)

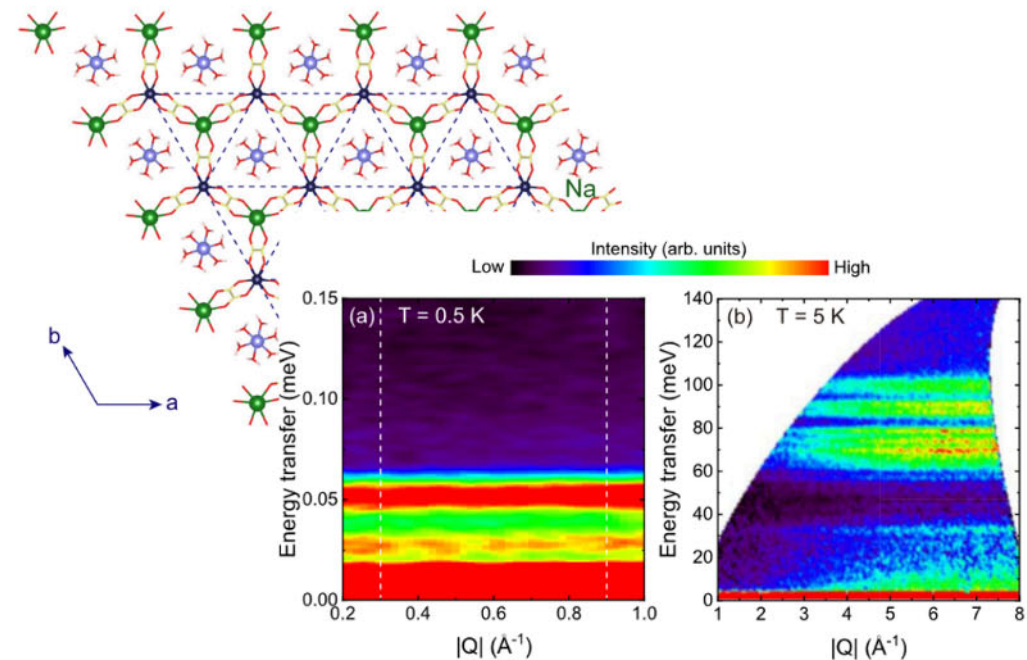
Broad dynamic and spatial range

PHYSICAL REVIEW B 103, 024402 (2021)



Direct determination of the zero-field splitting for the Fe^{3+} ion in a synthetic polymorph of $\text{NaMgFe}(\text{C}_2\text{O}_4)_3 \cdot 9\text{H}_2\text{O}$: A natural metal-organic framework

MOF: Abundant topological structures with broad prospects in gas storage and separation, catalysis ... chemical sensing



CNCS: $0 < \Delta E < 0.15$ meV: Magnetic modes
SEQUOIA: $60 < \Delta E < 120$ meV: Molecular vibrations of H_2O

TREX: The bispectral chopper spectrometer with PA.

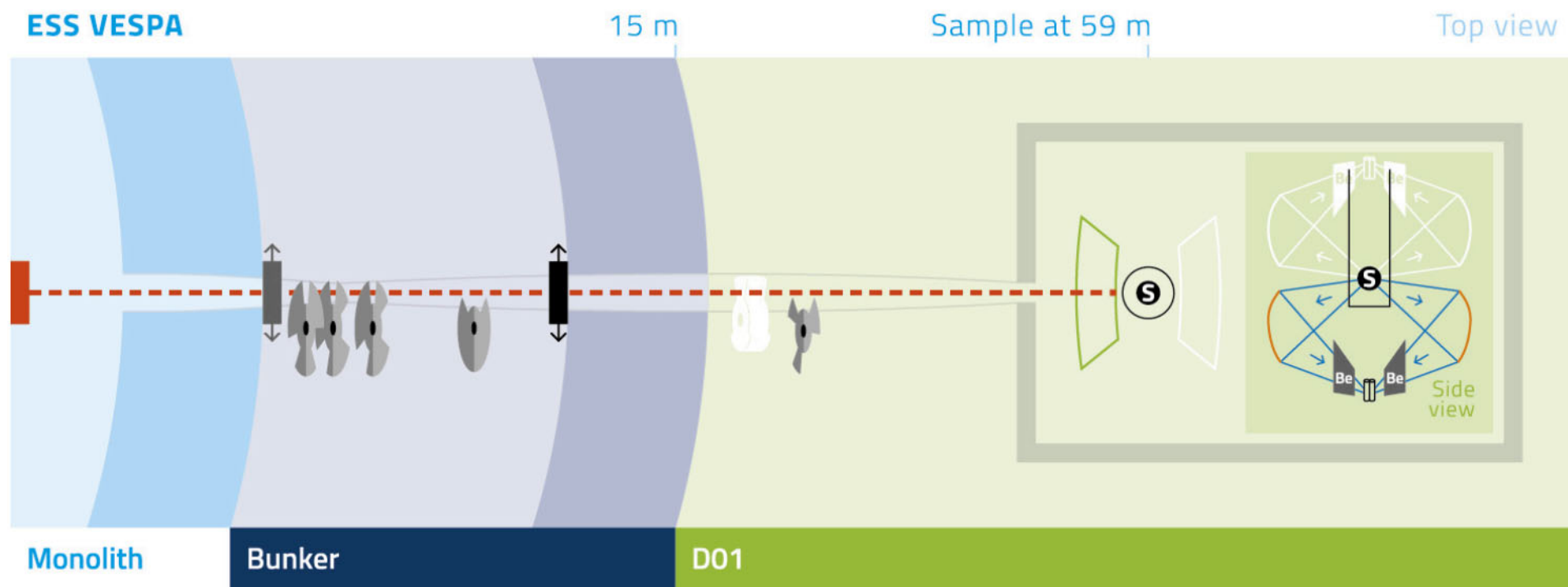


First Science workshop: November 2026

VESPA: The vibrational spectrometer of the ESS

Lead scientist: Adrien Perrichon, Monika Hartl

Lead instrument engineer: Rosa Camilleri Lledó & Liam Whitelegg:

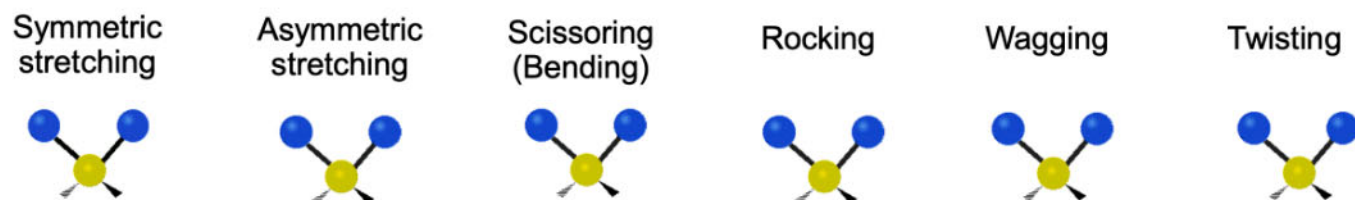


Neutron analogue to infrared/Raman
Quantitative, no selection rules, bulk

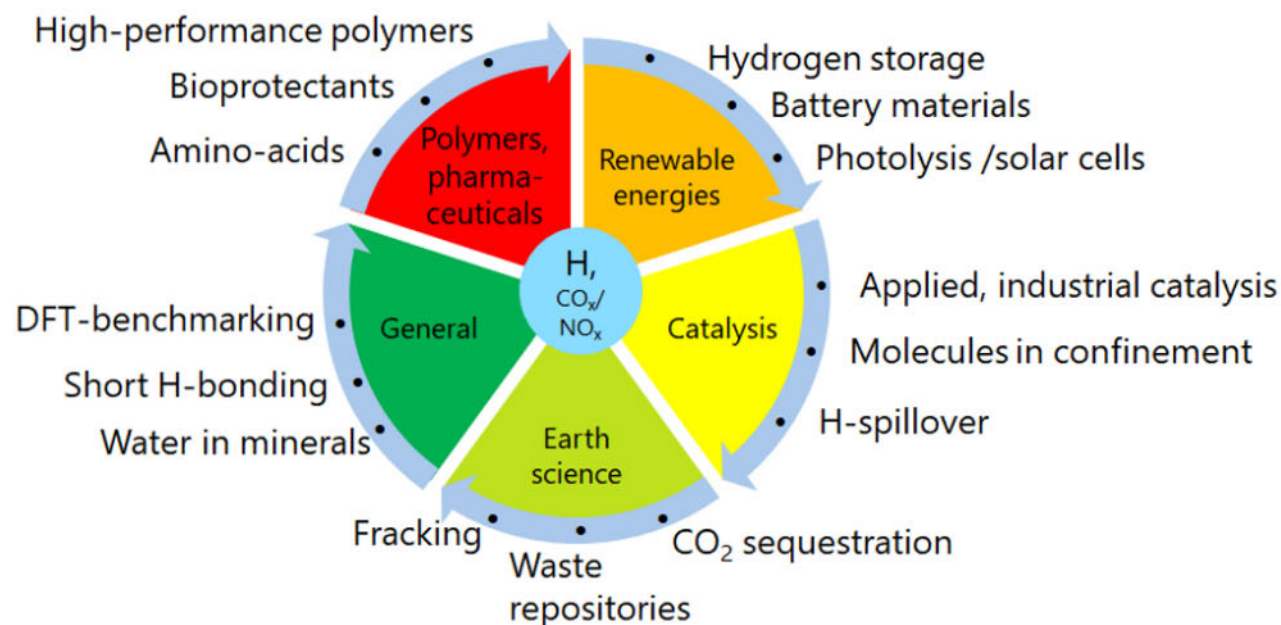
VESPA: The vibrational spectrometer of the ESS

Science case

VESPA optimised to study molecular vibrations (C-N, N-H & O-H)

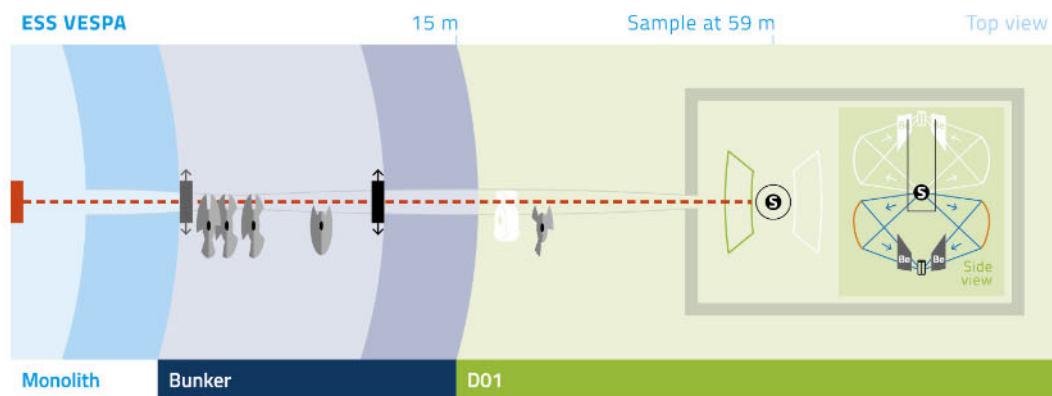


Broad science case in chemistry, focus on catalysis & energy materials



VESPA: The vibrational spectrometer of the ESS

In detailed design

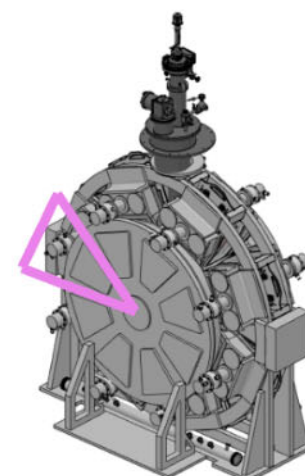
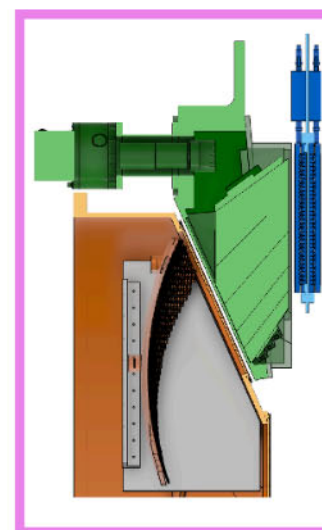


- Indirect-geometry crystal-analyser
- Moderator to sample distance: 59 m: $\Delta\lambda = 4.3 \text{ \AA}$.
- Direct view of the thermal moderator ($E_i = 3 - 500 \text{ meV}$)
- “Fingerprint” region: $480 - 1800 \text{ cm}^{-1}$ ($60 - 220 \text{ meV}$)
- Complex chopper cascade to achieve 3 subframes and variable resolution

Complex and compact secondary spectrometer:

280 ^3He tubes, 8500 HOPG crystals (7.0 sr), 200 kg of cryo-cooled Be, in vacuum vessel

Simultaneous diffraction, PDF & transmission



95% of measurements at base temperature ($<10\text{K}$) = fast cooling CCR always installed

90% of measurements <30 minutes in standard cans = high-capacity sample changer

VESPA: Vibrational spectrometer Enormous industrial impact Example from TOSCA at the ISIS Facility



communications
chemistry

JM Johnson Matthey
Inspiring science, enhancing life

ARTICLE

<https://doi.org/10.1038/s42004-021-00613-z> OPEN

Understanding the ZIF-L to ZIF-8 transformation
from fundamentals to fully costed kilogram-scale
production

Adam Deacon¹, Ludovic Briquet², Magdalena Malankowska^{3,4}, Felicity Massingberd-Mundy²,
Svermir Rudić⁵, Timothy I. Hyde², Hamish Cavaye⁵, Joaquín Coronas^{3,4}, Stephen Poulston² &
Timothy Johnson²



Catalysis Today

Volume 368, 15 May 2021, Pages 20–27



Neutron spectroscopy studies of methanol to hydrocarbons catalysis over ZSM-5

A. Zachariou^{a,c}, A. Hawkins^{a,c}, S.F. Parker^b, D. Lennon^c, R.F. Howe^d

LUCIDEON

Inelastic neutron scattering reveals the extent of active dissolution from Lucideon's iCRT platform technology

Angewandte
International Edition Chemie



A Journal of the
German
Chemical Society

Communication

Vibrational Analysis of an Industrial Fe-Based Fischer–Tropsch Catalyst Employing Inelastic Neutron Scattering[†]

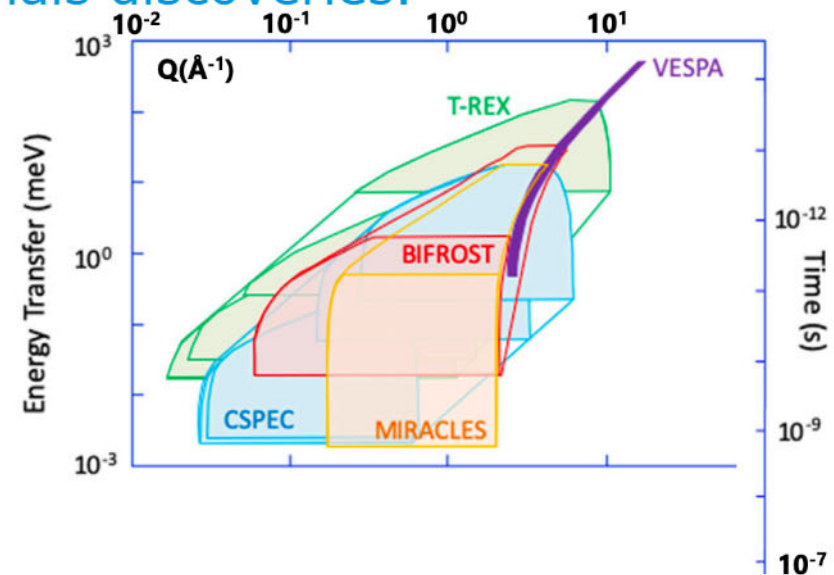
Dr. Neil G. Hamilton, Dr. Ian P. Silverwood, Robbie Warringham, Dr. Josef Kapitán, Dr. Lutz Hecht,
Dr. Paul B. Webb Prof. Robert P. Tooze, Dr. Stewart F. Parker, Dr. David Lennon

First published: 16 April 2013 | <https://doi.org/10.1002/anie.201210179> | Citations: 25

In conclusion: Spectroscopy division Addressing needs for materials discoveries.

- 1) CSPEC (2027)
- 2) BIFROST (BOT, 2026)
- 3) MIRACLES (2027)
- 4) T-REX (2027)
- 5) VESPA (2028)

NSE/Backscattering/Broad bandwidth TOF?



Long pulse: Spectroscopy: Opportunities from Reactor & Spallation facilities

High signal (long pulse) to noise (spallation)

Wavelength band - broad (short instruments), focussed (long instruments)

$S(\mathbf{Q}, \omega)$: Broad with Unparalleled energy resolution nano to meV: trade energy for flux.

Strength of neutrons: $S(\mathbf{Q}, \omega)$ - Born approximation. Optimise work flow from data to understanding (DMSC)

Routine:

Polarisation Analysis

Time dependent phenomena

Efficient screening and discovery of new mater

Building the Spectroscopy division at ESS



*CLOSE COLLABORATION WITH COMMUNITY VIA AFFILIATE POSITIONS,
COLLABORATIONS & IN-KIND PARTNERS*

PASCALE.DEEN@ESS.EU