T-REX
Time-of-flight Reciprocal space Explorer

A neutron spectrometer for
magnetism,
material science,
soft matter
at ESS

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Basic properties of thermal neutrons

"A gentle probe for condensed matter"

…

Cold neutrons	$0.5 \lesssim E \lesssim 5$	meV
• Thermal neutrons	$5 \lesssim E \lesssim 100$	meV
Hot neutrons	$100 \lesssim E \lesssim 500$	meV
Epithermal neutrons	$500 \lesssim E \lesssim 1000$	meV

…

- "Thermal" $E \cong 25\ \text{meV} \quad \Rightarrow \quad T = \frac{E}{k_B} \cong 293\ \text{K}$

Boltzmann constant: $k_B \cong 8.167 \times 10^{-5}\ \text{eV}\cdot\text{K}^{-1}$

Basic properties of thermal neutrons

"A gentle probe for condensed matter"

- Peculiar value of the neutron mass: $m \cong 1.675 \times 10^{-27}$ kg

Energy $E = \frac{1}{2} m v^2 \cong 25$ meV ~ excitations energies in condensed matter dynamics

Speed $v = \sqrt{\frac{2E}{m}} \cong 2200$ m/s

Wavelength $\lambda = \frac{h}{mv} \cong 1.8$ Å ~ interatomic distances in condensed matter structure

Wavevector $k = \frac{2\pi}{\lambda} \cong 3.5$ Å^{-1} $\Rightarrow$ $E = \frac{\hbar^2 k^2}{2m}$

Planck constant: $h \cong 4.136 \times 10^{-15}$ eV·s Reduced Planck constant: $\hbar = h/2\pi \cong 0.658 \times 10^{-15}$ eV·s

Basic properties of thermal neutrons

"A gentle probe for condensed matter"

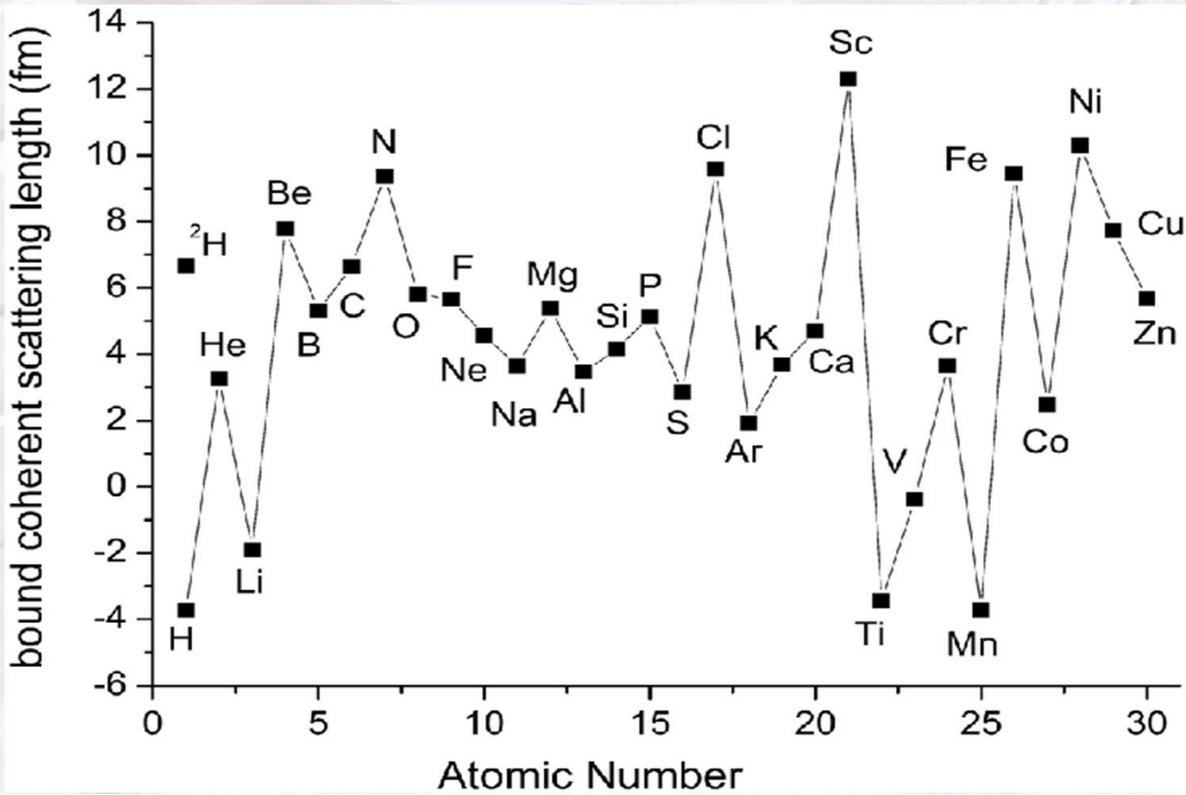
- Zero electric charge

⇒ Interaction with nuclei via nuclear forces

"weak" coupling, penetrate deeply and get close to the nuclei

⇒ bulk samples

⇒ sensitive to nuclides and isotopes



Basic properties of thermal neutrons

"A gentle probe for condensed matter"

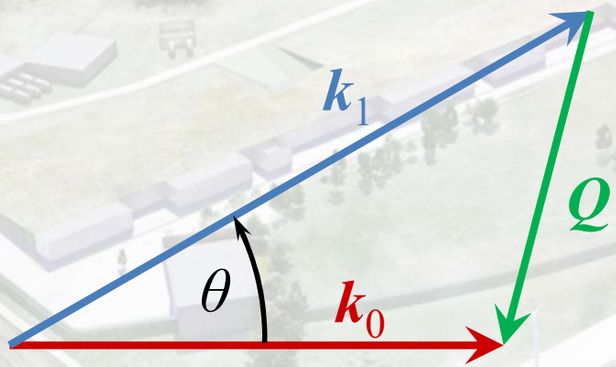
- Spin $\frac{1}{2}$ and magnetic moment

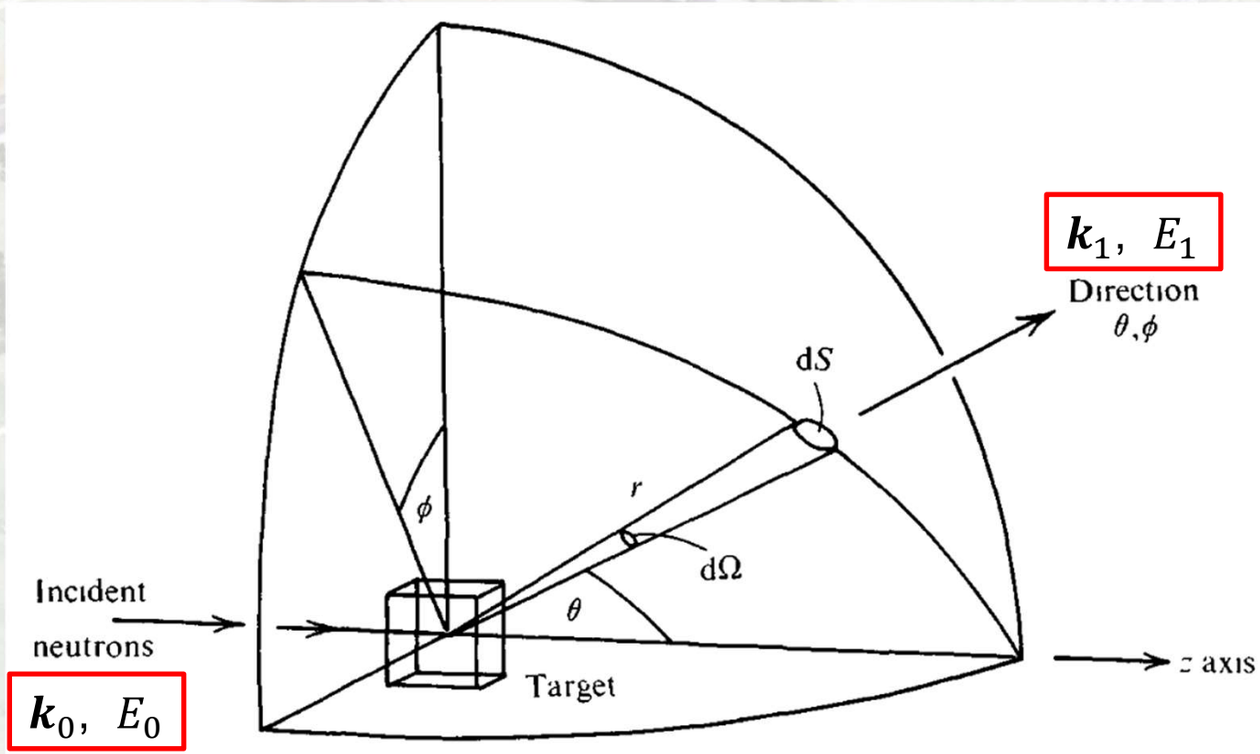
  ⇒ Interaction with unpaired electrons of magnetic atoms

  structure and dynamics of magnetic systems

Double differential cross-section

$$\left(\frac{d^2\sigma}{d\Omega dE_1}\right) = \frac{k_1}{k_0}\frac{1}{2\pi\hbar}\sum_{ij} b_i b_j \int_{-\infty}^{\infty} \left\langle e^{-i\boldsymbol{Q}\cdot\boldsymbol{R}_i(0)}\, e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)} \right\rangle e^{-i\omega t}\, dt$$





Double differential cross-section

$$\left(\frac{d^2\sigma}{d\Omega dE_1}\right) = \frac{k_1}{k_0}\frac{1}{2\pi\hbar}\sum_{ij} b_i b_j \int_{-\infty}^{\infty} \left\langle e^{-i\boldsymbol{Q}\cdot\boldsymbol{R}_i(0)}\, e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)} \right\rangle e^{-i\omega t}\, dt$$

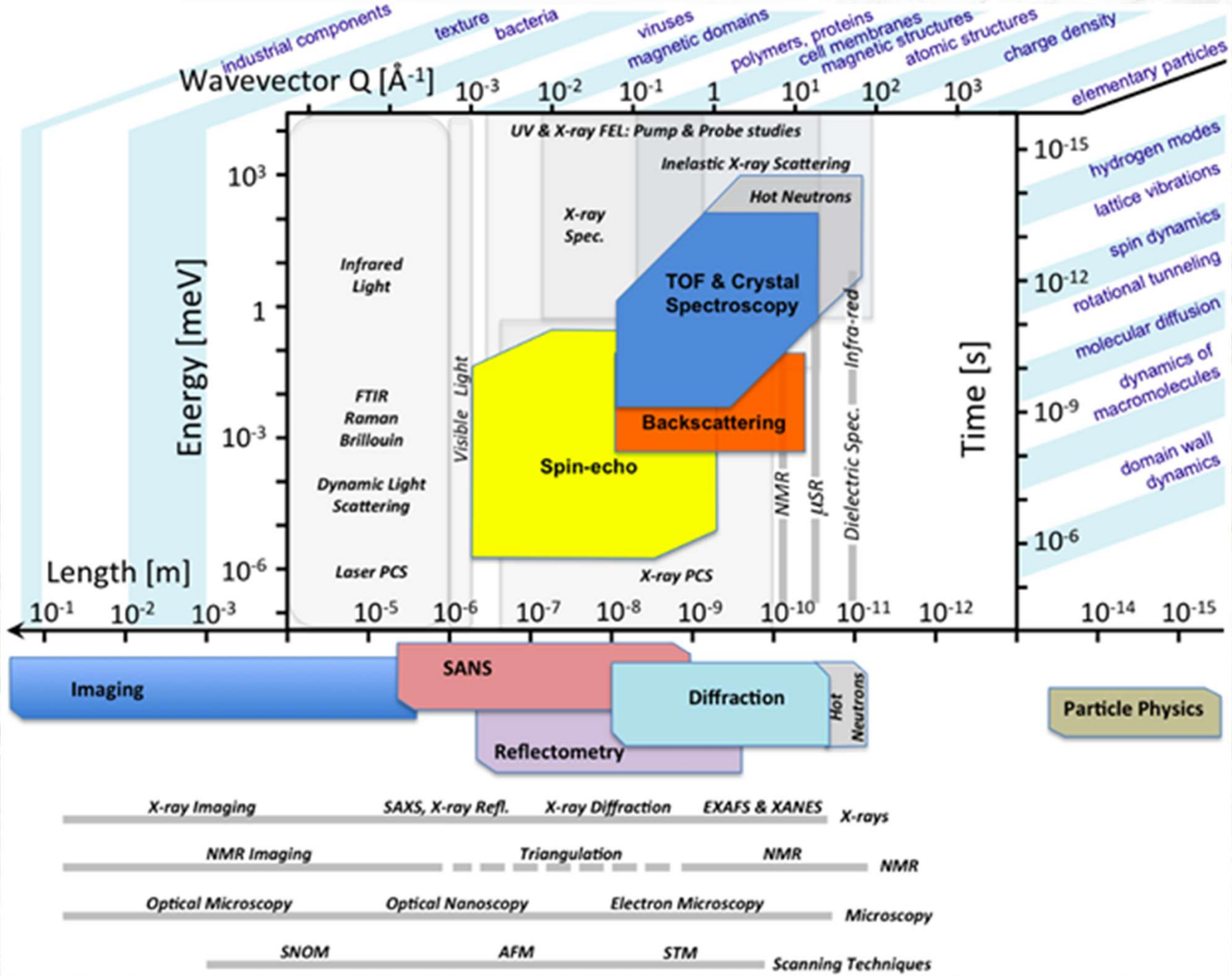
Neutron flux and kinematics

Coupling

Sample Properties !
$\boldsymbol{R}_i(0), \boldsymbol{R}_j(t)$
where atoms ARE
what atoms DO

STRUCTURE and DYNAMICS

Thermal Neutrons



Thermal Neutrons

An excellent probe for condensed matter

PROS

- Thermal (300 K) $\Rightarrow$ $\lambda \sim$ Å, $E \sim$ meV
  atomic structure & dynamics
- Spin $\Rightarrow$ magnetic structure & dynamics
- No charge (“a gentle probe”)
  $\Rightarrow$ weak coupling, linear response, bulk probe
- Coherent and incoherent scattering
  $\Rightarrow$ both collective and single-particle dynamics
- Isotope substitution $\Rightarrow$ atom selective investigations

CONS

- No charge $\Rightarrow$ bulk samples: big samples, no surface
- Need a Large Infrastructure for the SOURCE!!

Neutrons: a European Leadership

- ILL — Grenoble (France) — *continuous*
- ISIS — Abingdon (United Kingdom) — *pulsed*
- FRM2 — Munich (Germany) — *continuous*
- PSI — Villigen (Switzerland) — *pulsed*

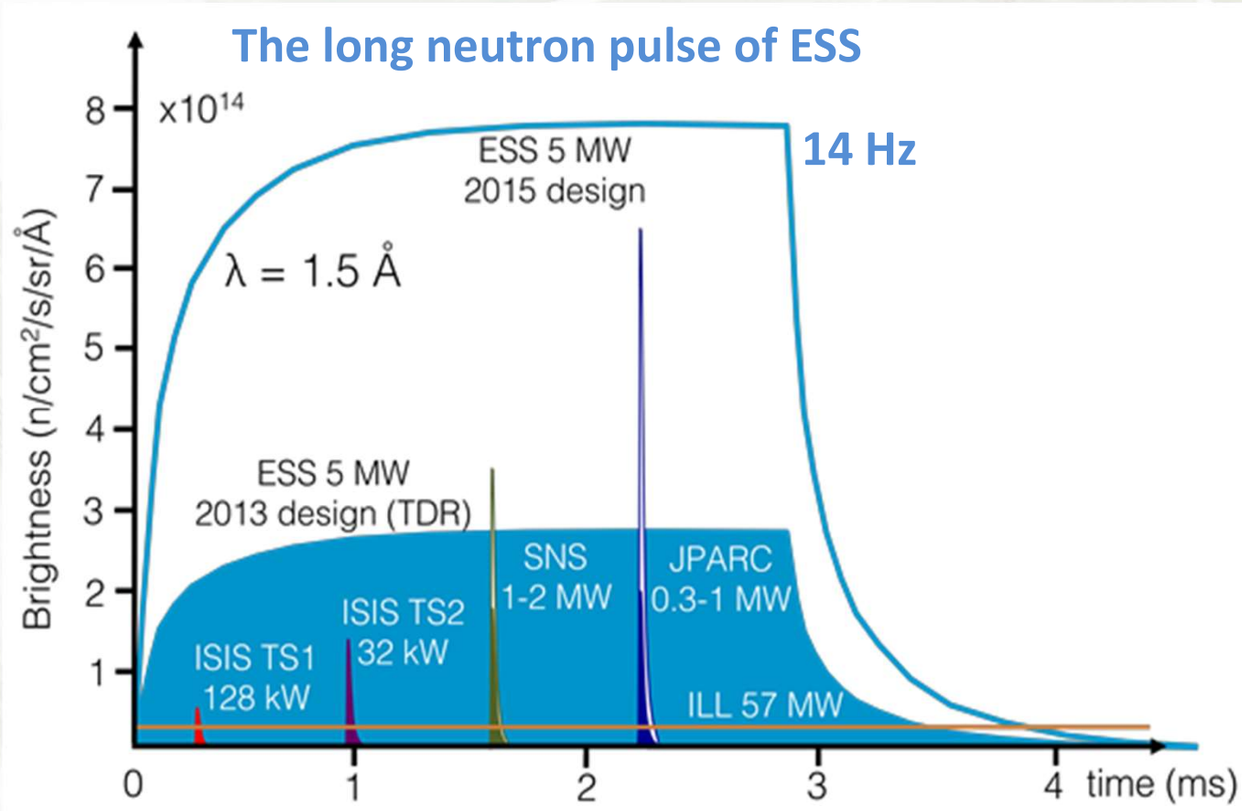
- SNS — Oak Ridge (US)
- J-PARC — Tokai (Japan)
- Ansto — Lucas Heights (Australia)
- CSNS — Dongguan (China)

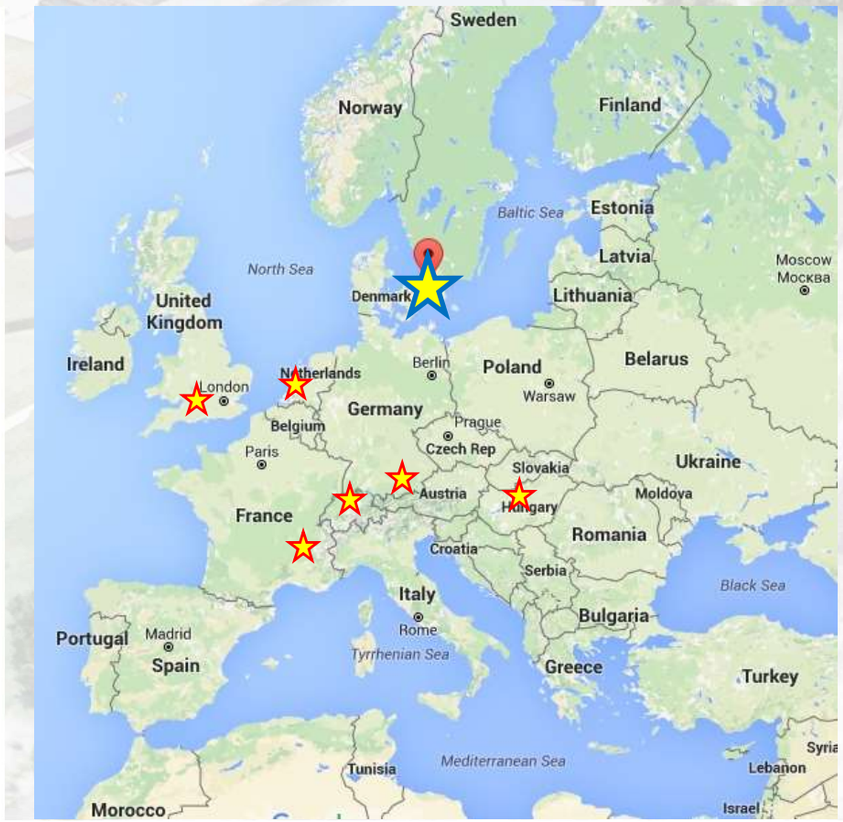


European Spallation Source

(*Lund,* Sweden)

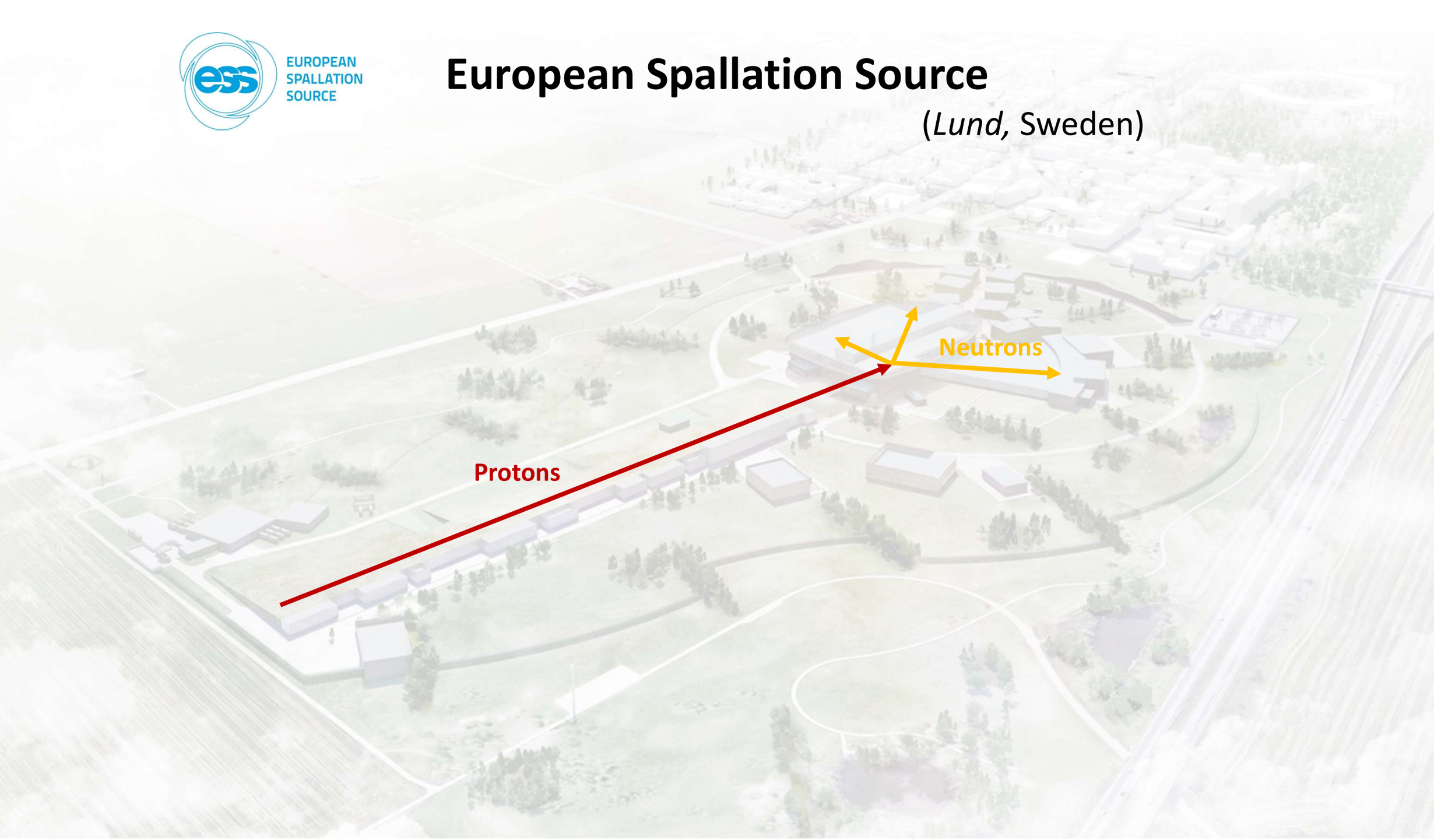
- New-generation pulsed neutron source
- Higher brightness
- World-leading neutron facility





European Spallation Source

(*Lund,* Sweden)



The In-Kind Contribution process

- Started in 2011
- 14 in-kind partner countries nowadays
- Call for in-kind proposals (2012)
- Collection of proposals from partner countries for:
  - Conventional facilities
  - Accelerator
  - Target
  - Neutron instruments
- Thorough selection of proposals
  (still ongoing!)
- Progressive acceptance of proposals and in-kind values:
  - 15 out of 22 instruments

→ T-REX 16.85 M€ (2015)

→ VESPA 11.95 M€ (2016)




August 2017
170 m


April 2019

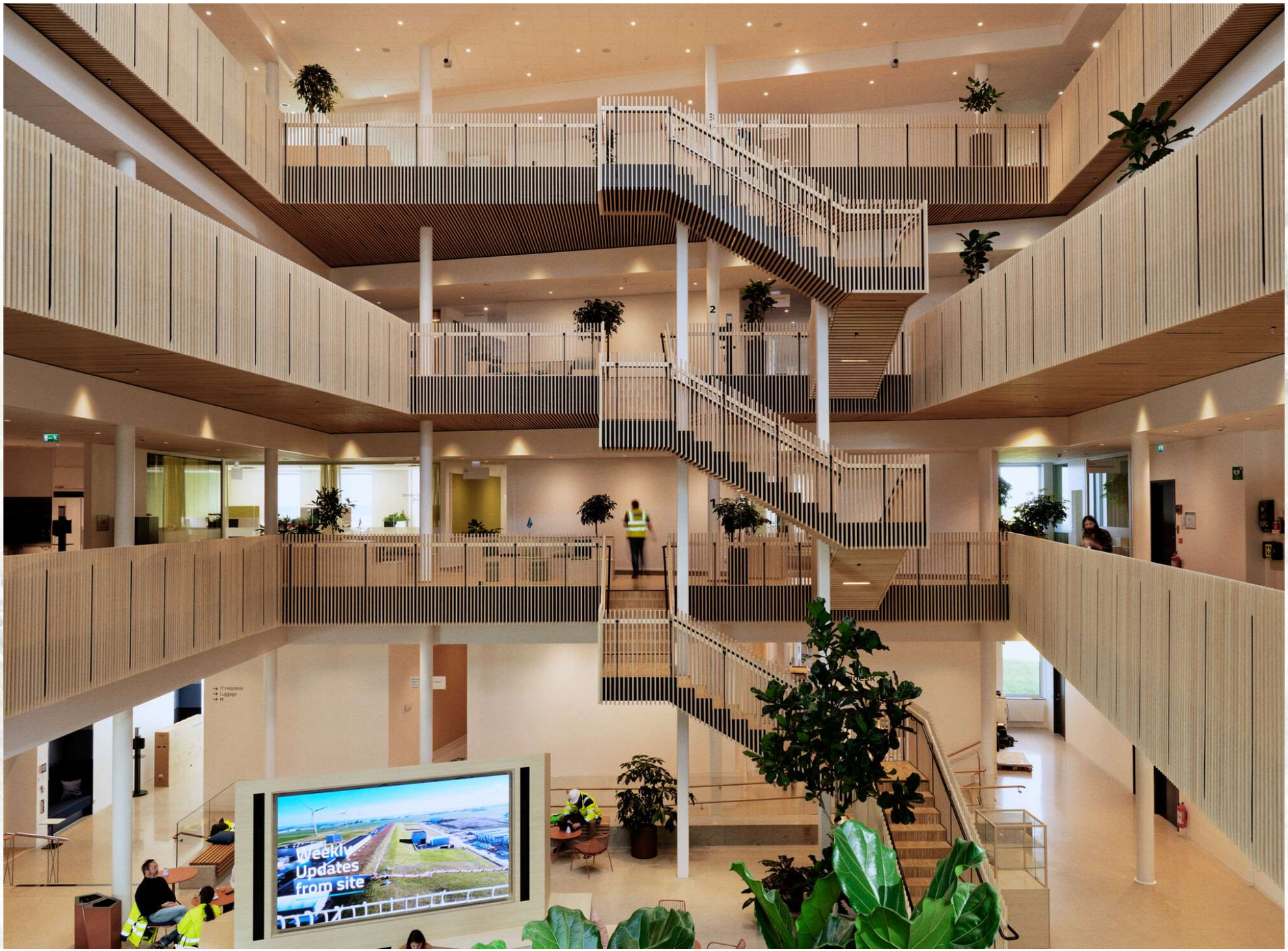

January 2021


November 2021

ESS in March 2024






Weekly
Updates
from site

T-REX

a German-Italian collaboration

Jülich Center for Neutron Science (Germany)


Thomas Brückel


Nicolò Violini


Christian Franz


Mario Könen


Tadeusz Kozielewski


Jörg Voigt


Marcel Serwe

~75%



~25%



CNR - IOM & Università degli Studi di Perugia (Italy)


Alessio Laloni


Andrea Orecchini


Francesco Sacchetti


Marco Zanatta


Enrico Zanieri


Gianluigi Piluso

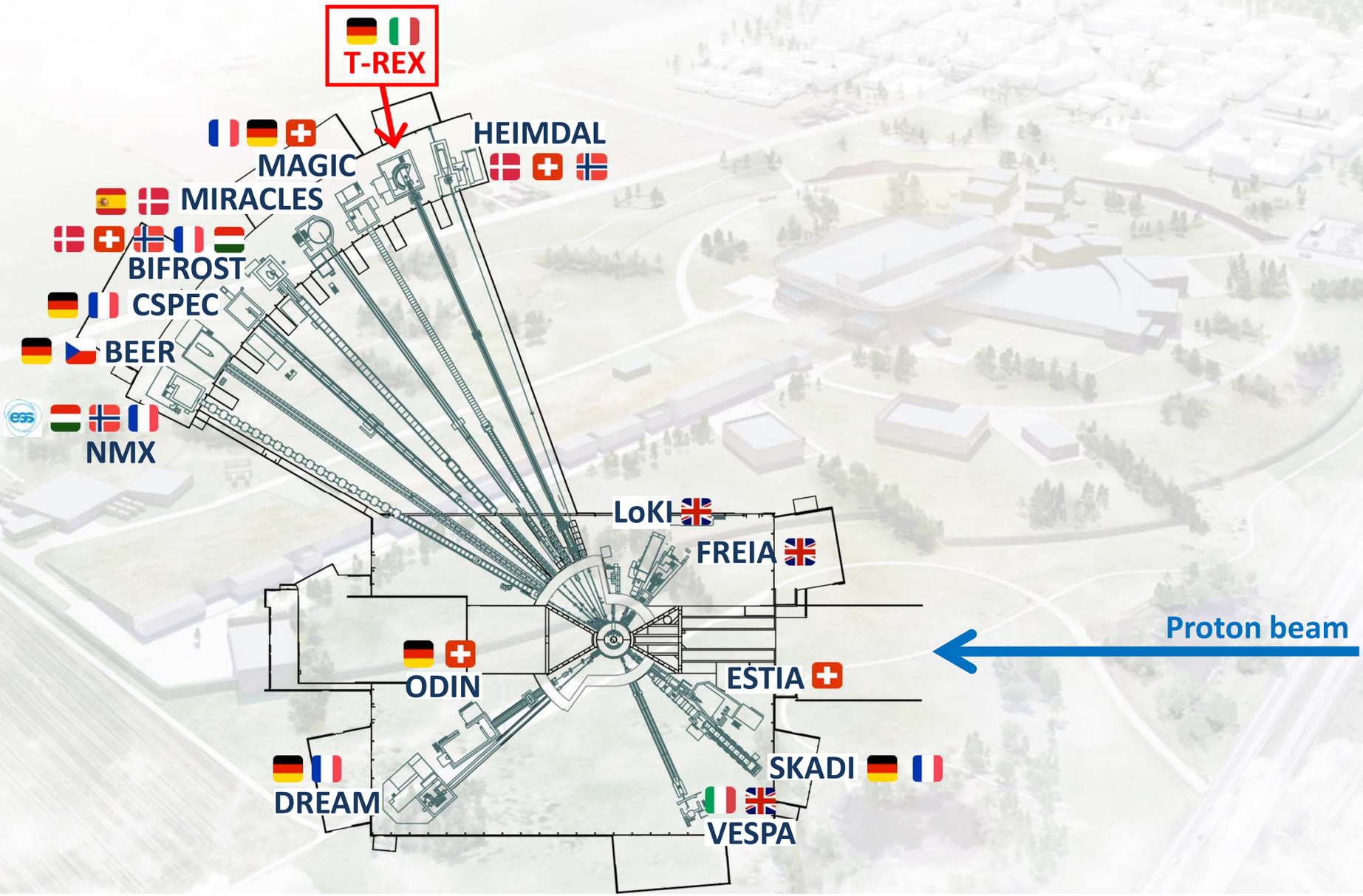

Lucia Comez


Pietro Tozzi

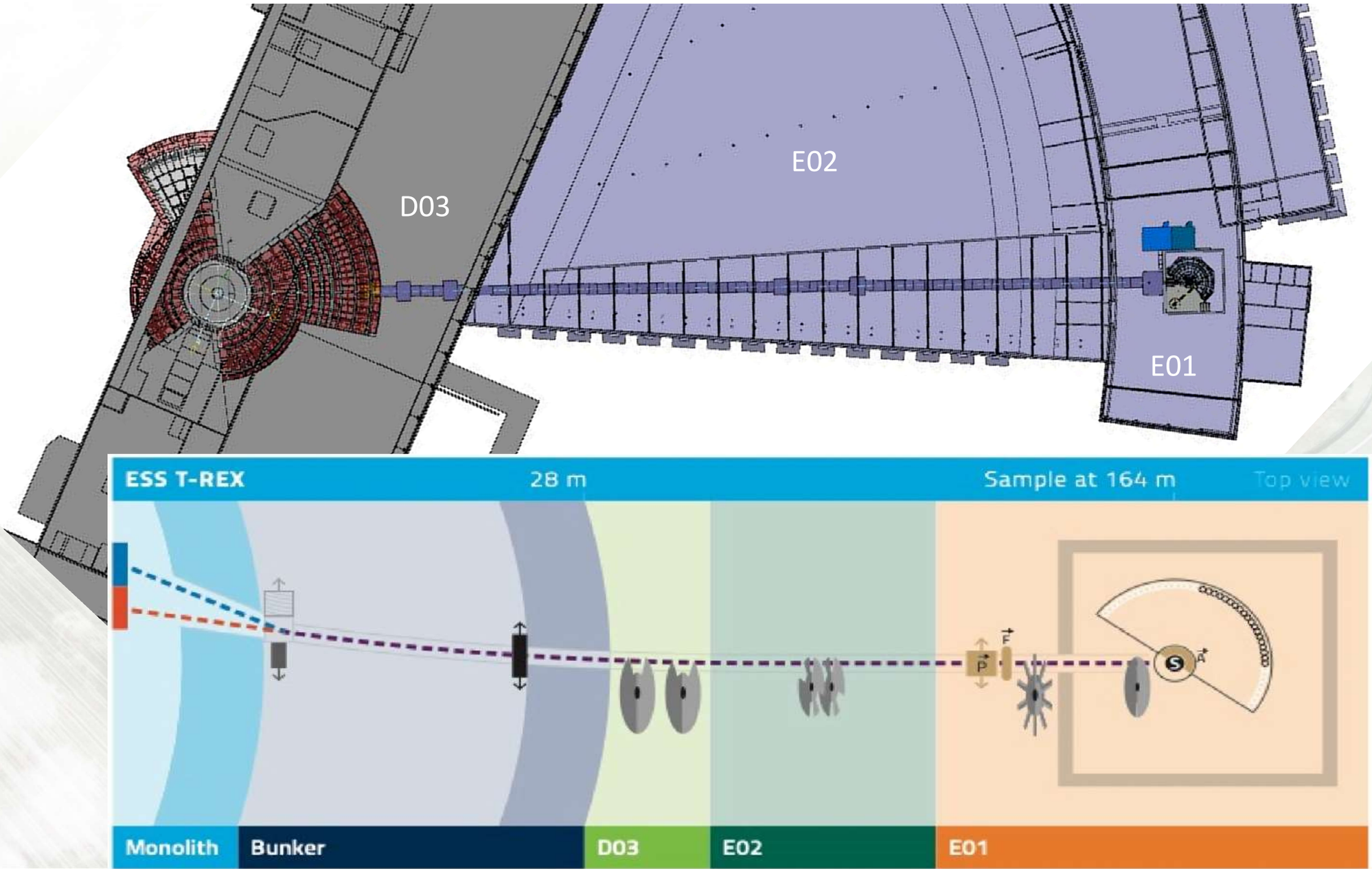

Alessandro Paciaroni


Gianluca Gubbiotti

T-REX within the ESS instrument suite

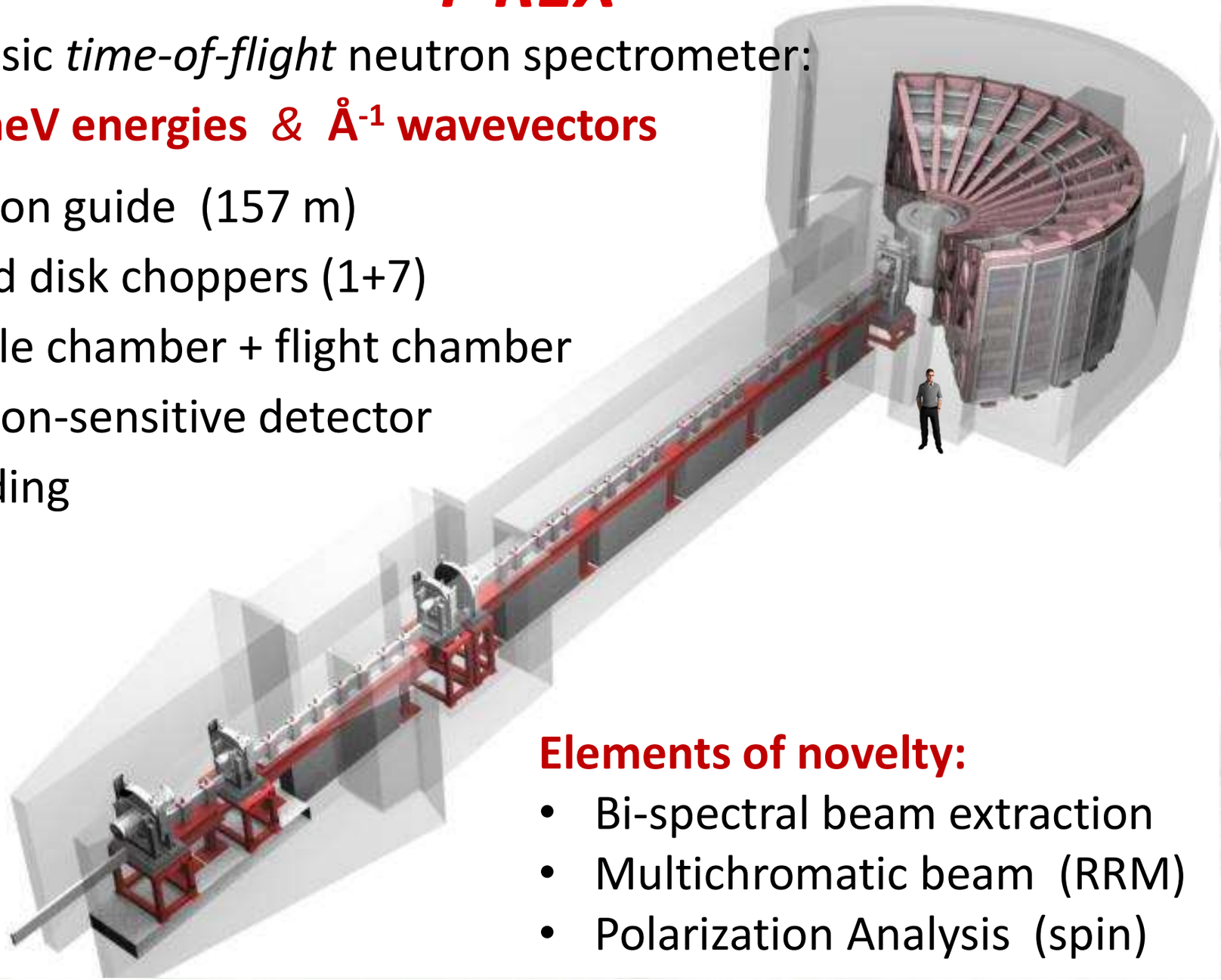


T-REX layout


D03
E02
E01
ESS T-REX
28 m
Sample at 164 m
Top view
Monolith
Bunker
D03
E02
E01

T-REX

- A classic *time-of-flight* neutron spectrometer:
- **meV energies & Å^{-1} wavevectors**
- neutron guide (157 m)
- T_0 and disk choppers (1+7)
- sample chamber + flight chamber
- position-sensitive detector
- shielding

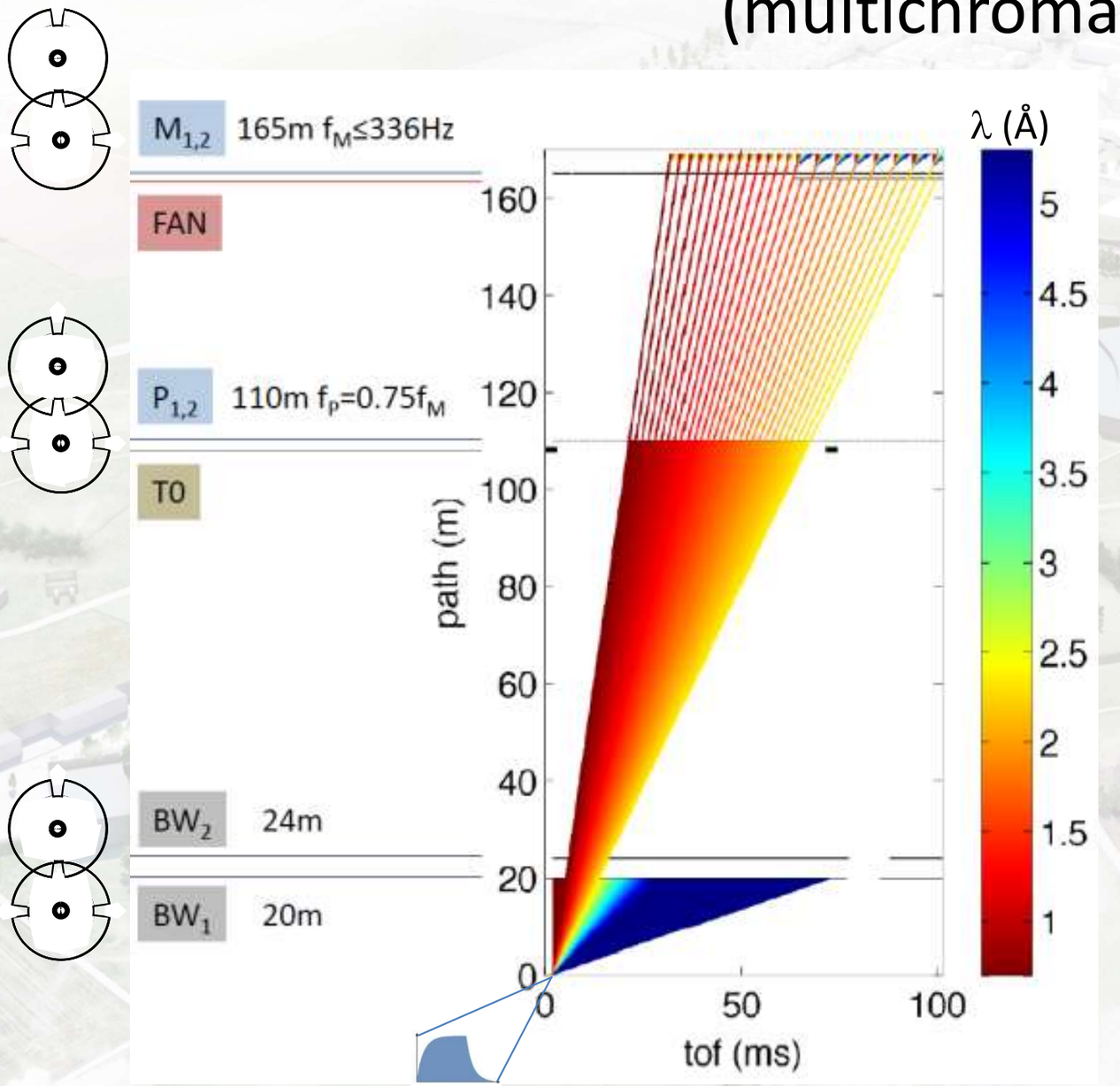


Elements of novelty:

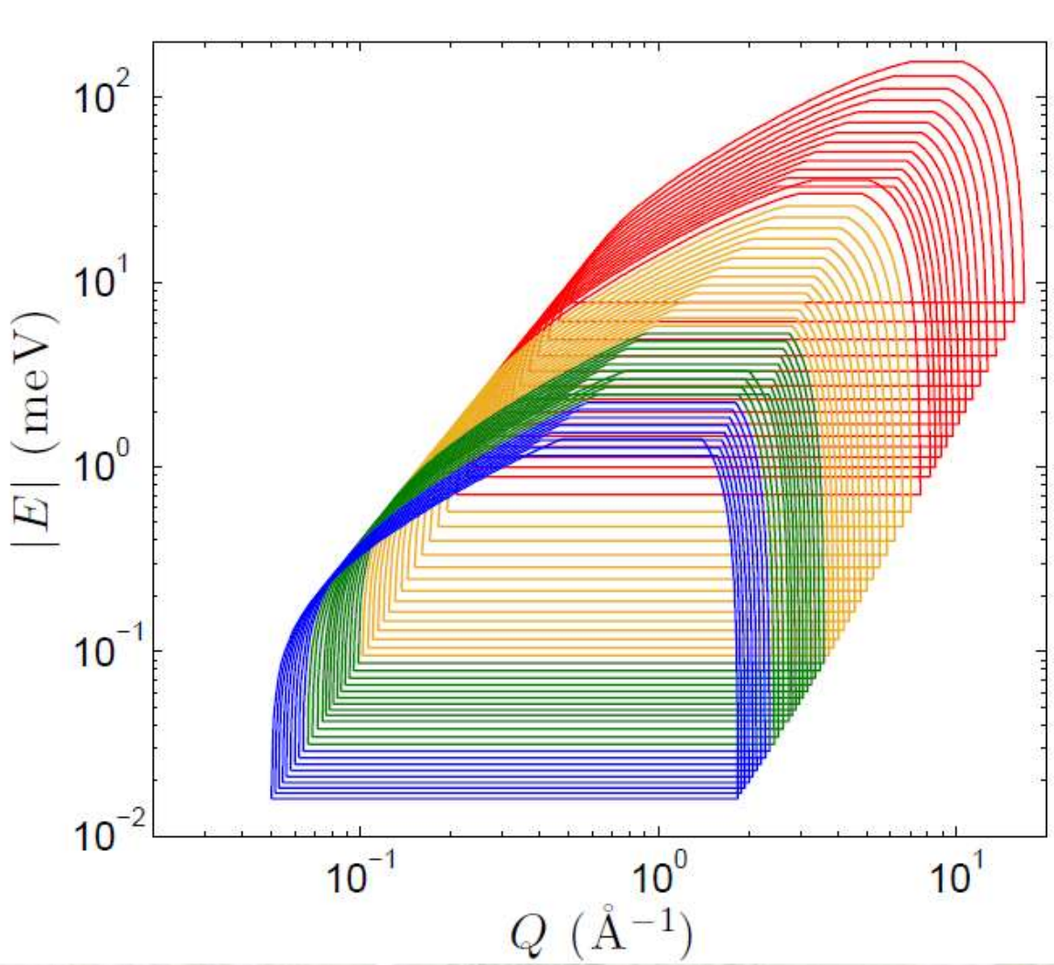
- Bi-spectral beam extraction
- Multichromatic beam (RRM)
- Polarization Analysis (spin)

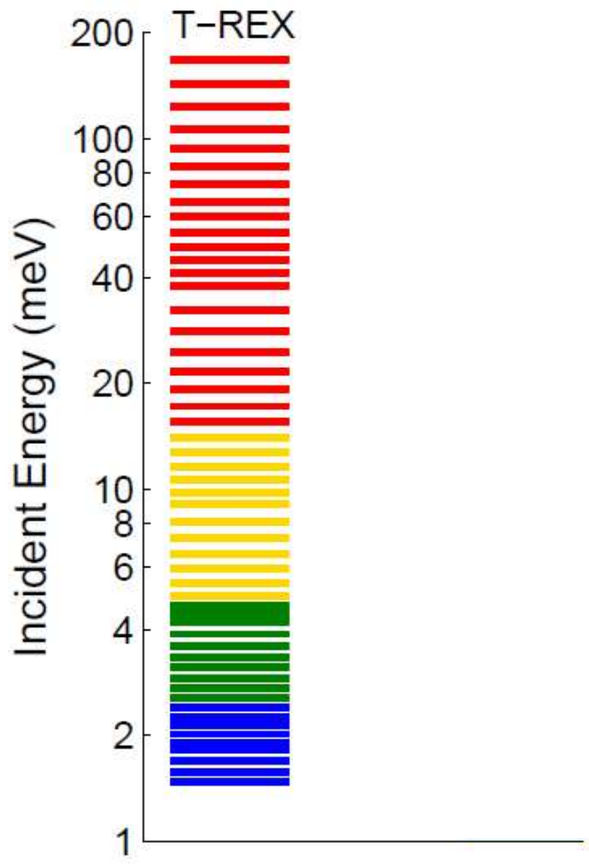
Time-Distance diagram

(multichromatic beam)



Dynamical Range





Main features

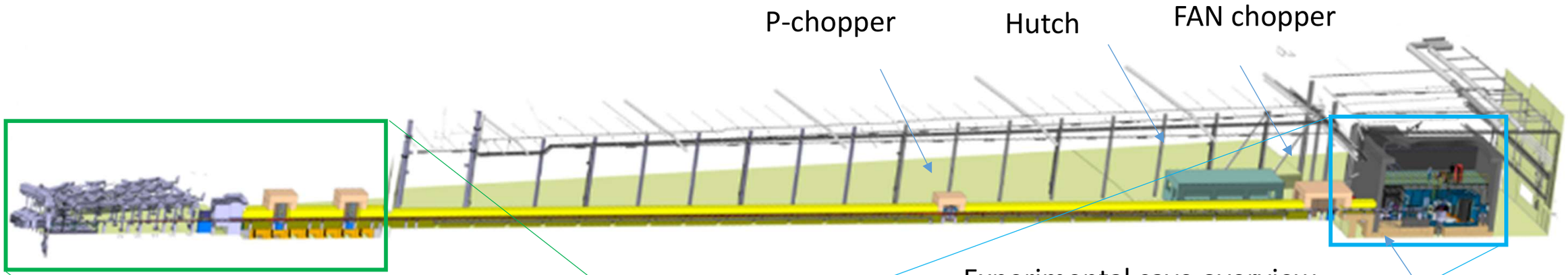
Incident energy	$2 < E < 160$ meV
Energy resolution	$0.02 < \Delta\hbar\omega < 10$ meV
Wavevector transfer range	$0.5 < Q < 170$ nm^{-1}
Wavevector transfer resolution	$0.1 < \Delta Q < 1$ nm^{-1}
Sample cross section	$\leq 10 \times 30$ mm^2
Main features	• Polarization analysis as a standard tool • Repetition rate multiplication • Four dimensional mapping capabilities • High intensity with low background • Adjustable resolution, for flexible trading of resolution for flux • Complex sample environment for *in-situ* and *in-operando* studies

Gain factors

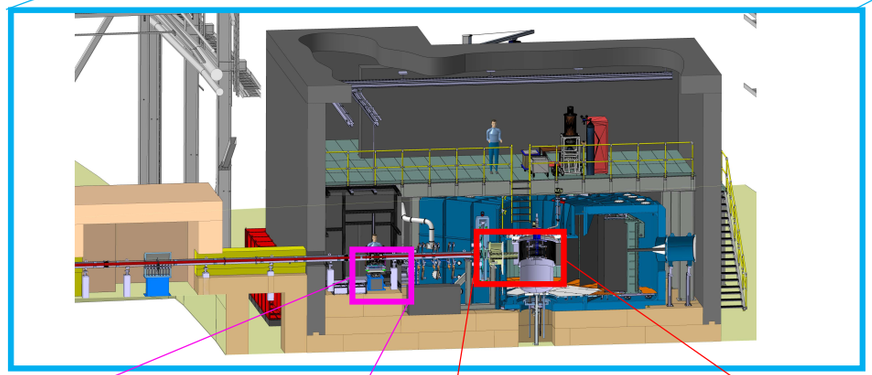
Instrument / T-REX gain factor	LET	IN5	CNCS	4-SEASONS
Monochromatic gain factor	38	9	9	9
Gain factor at maximal RRM	90	100	140	45

About ONE or TWO orders of MAGNITUDE

T-REX layout

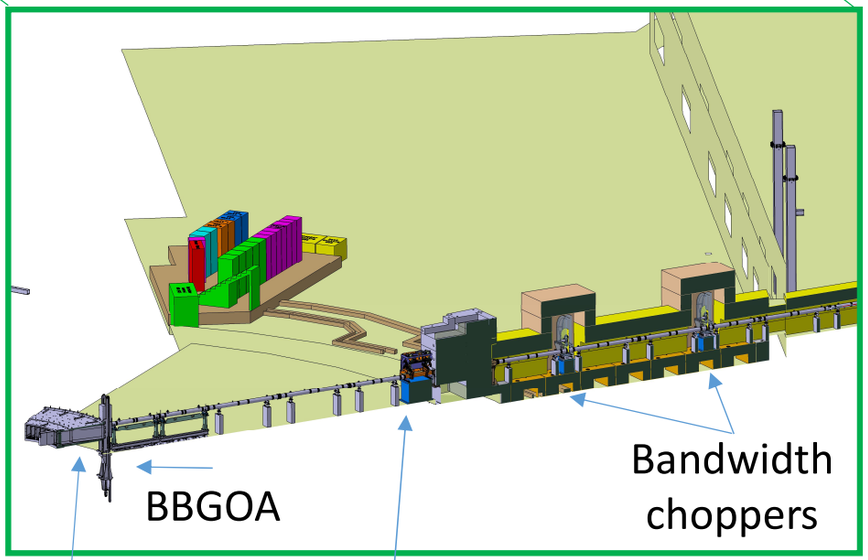


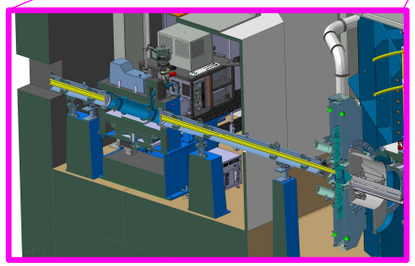
Experimental cave overview



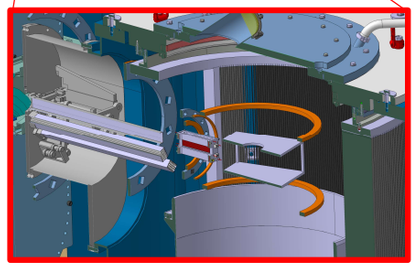
M-chopper

In-bunker + D03 building



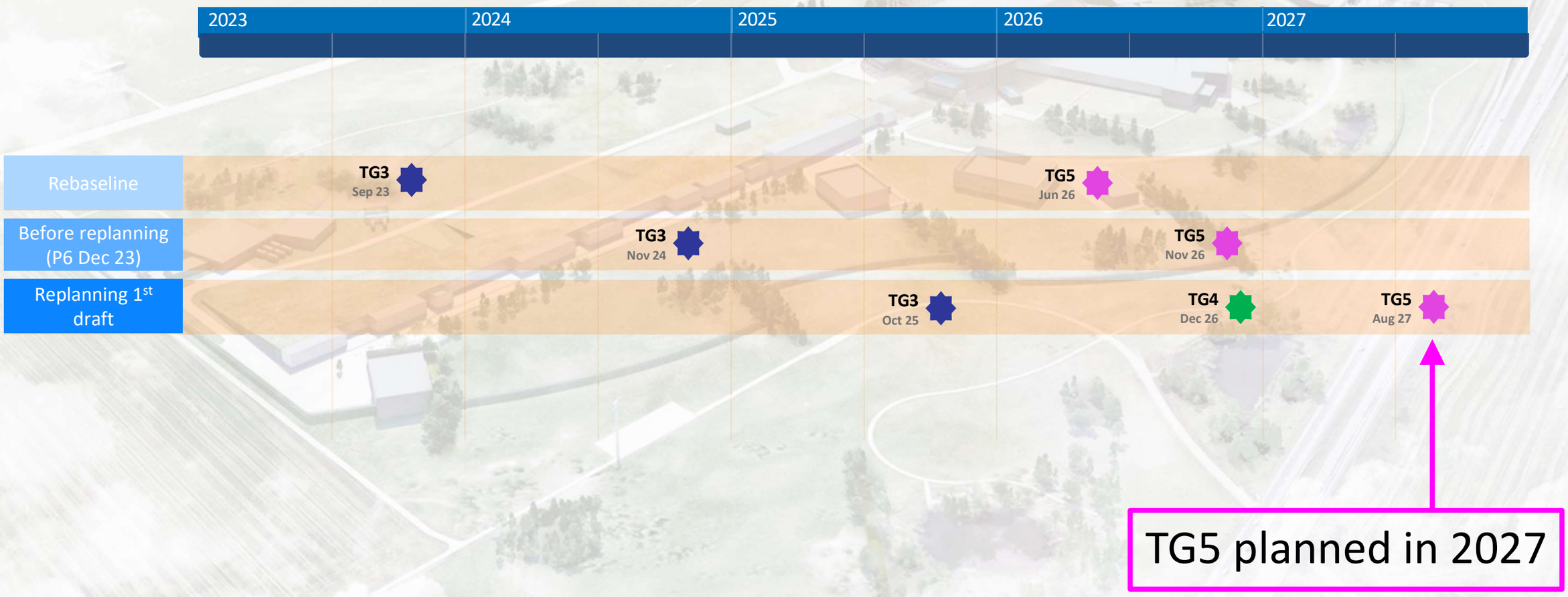


Therm. & cold polariser

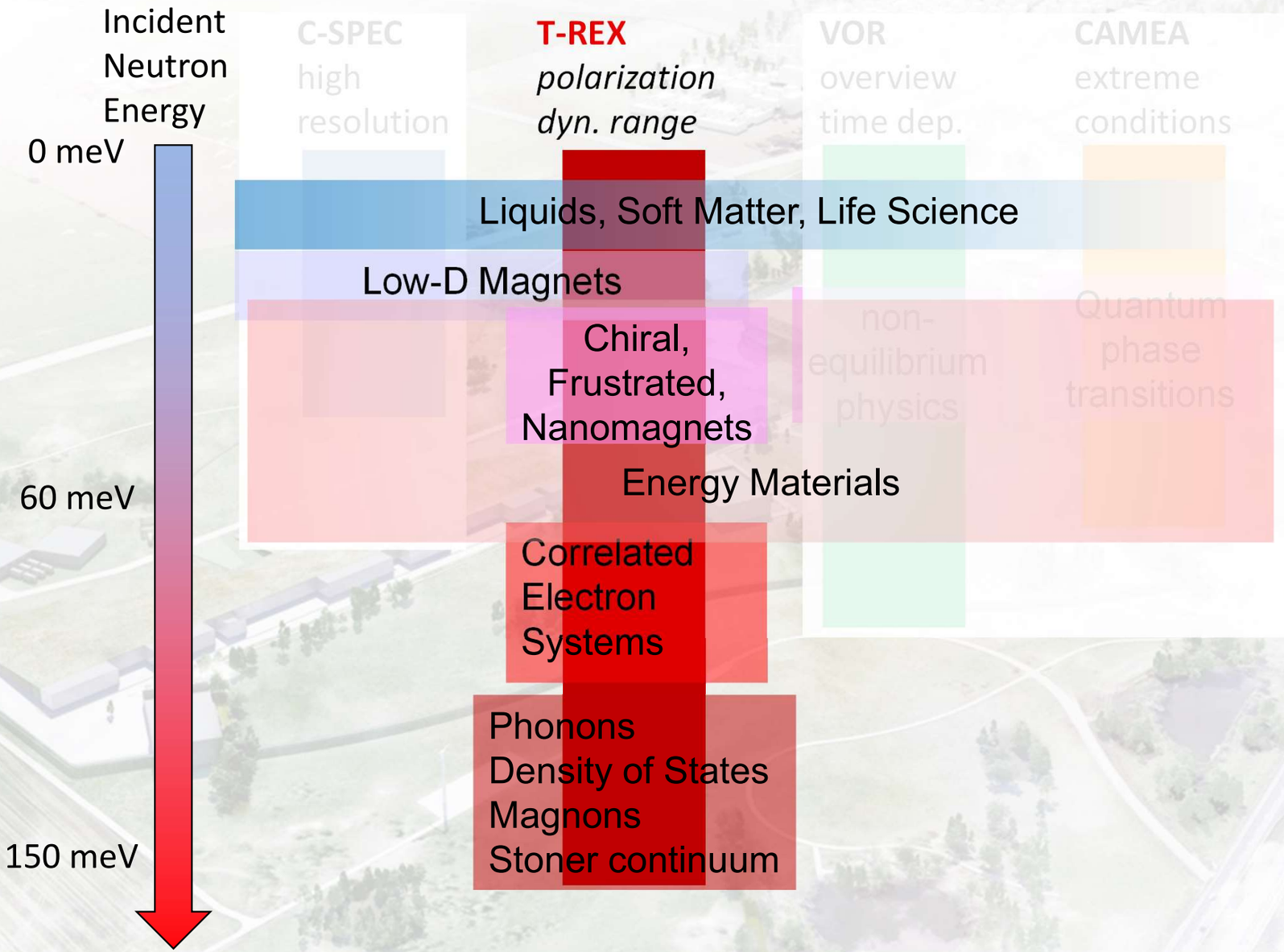


Primary collimator

Timeline


2023
2024
2025
2026
2027
Rebaseline
TG3
Sep 23
TG5
Jun 26
Before replanning (P6 Dec 23)
TG3
Nov 24
TG5
Nov 26
Replanning 1st draft
TG3
Oct 25
TG4
Dec 26
TG5
Aug 27
TG5 planned in 2027

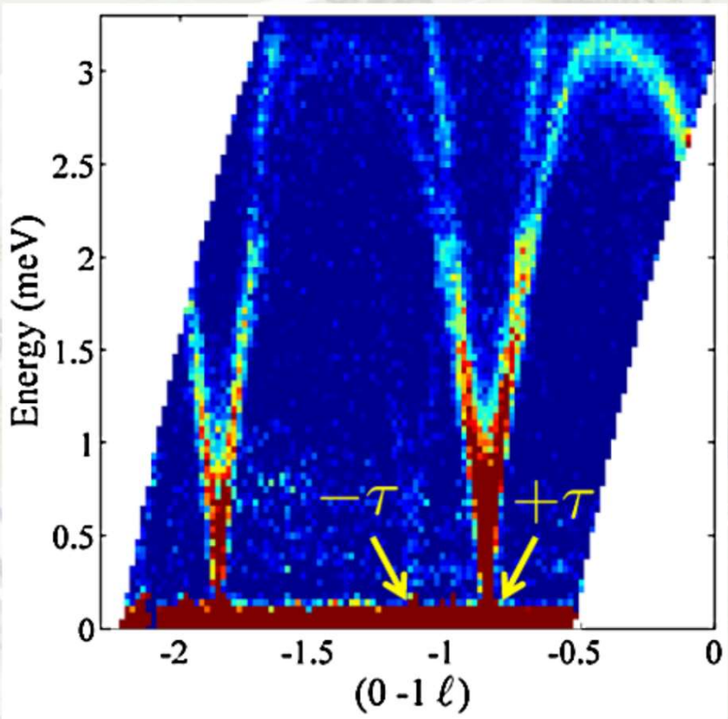
Science Cases



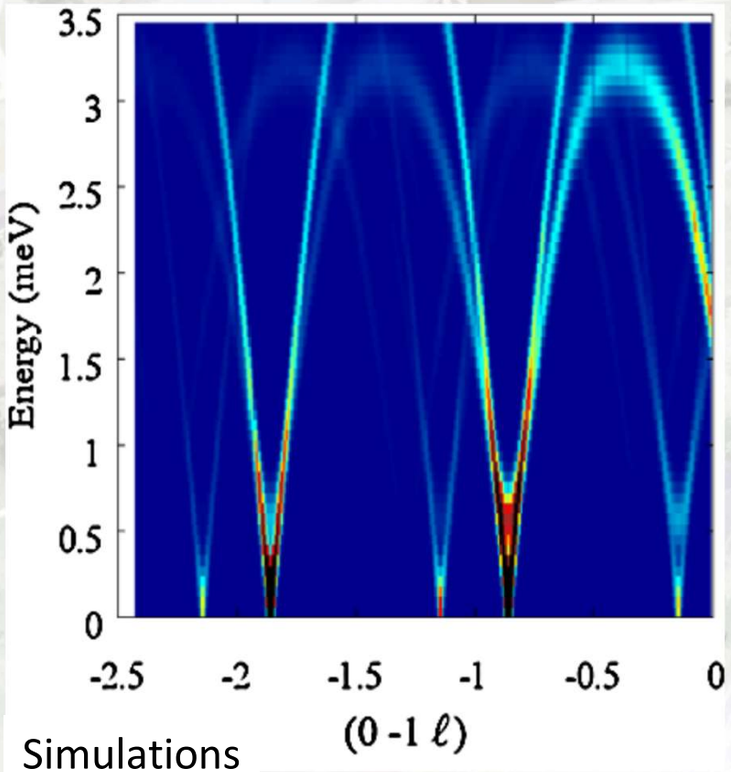
Spin waves in $Ba_3NbFe_3Si_2O_{14}$ single crystals

- Wide survey on IN5 (ToF) + Polarization Analysis on IN20 (TAS)

- Very good energy resolution
- Good ***Q*** resolution
- High flux



Expt. Data



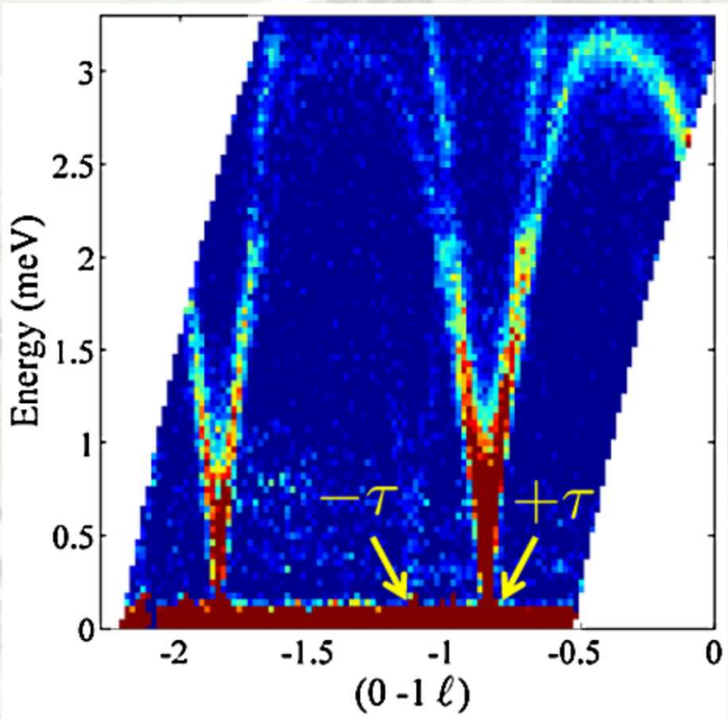
Simulations

Loire *et al.*, PRL **106**, 207201 (2011)

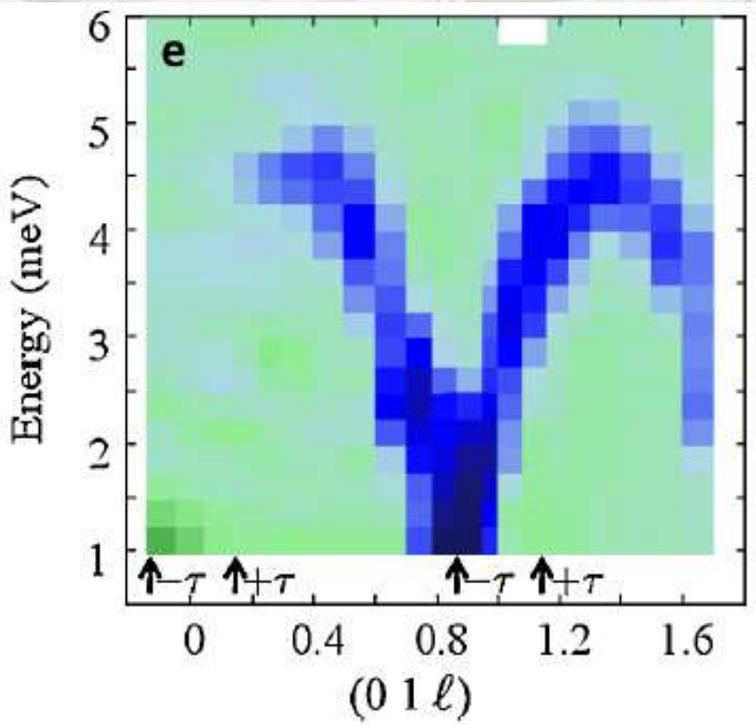
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Expt. Data

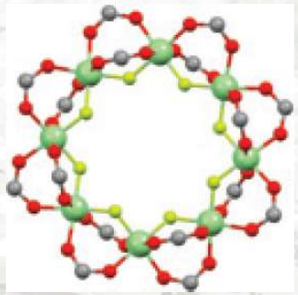


Expt. Data with Polarization Analysis

Loire *et al.*, PRL **106**, 207201 (2011)

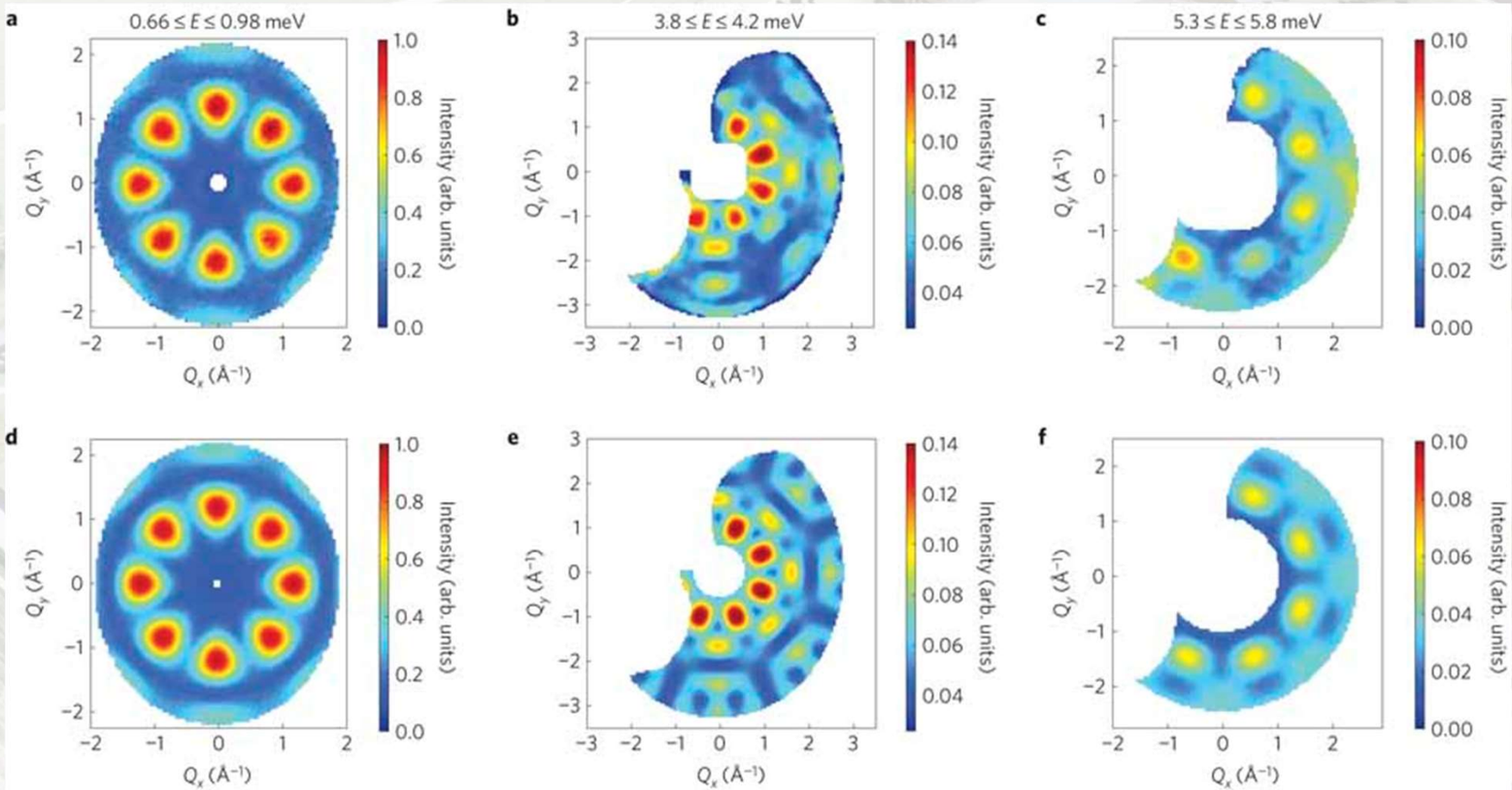
Spin dynamics of molecular nanomagnets

- Entangled spin states (quantum computing)
- Wide 4D mapping



data

fit



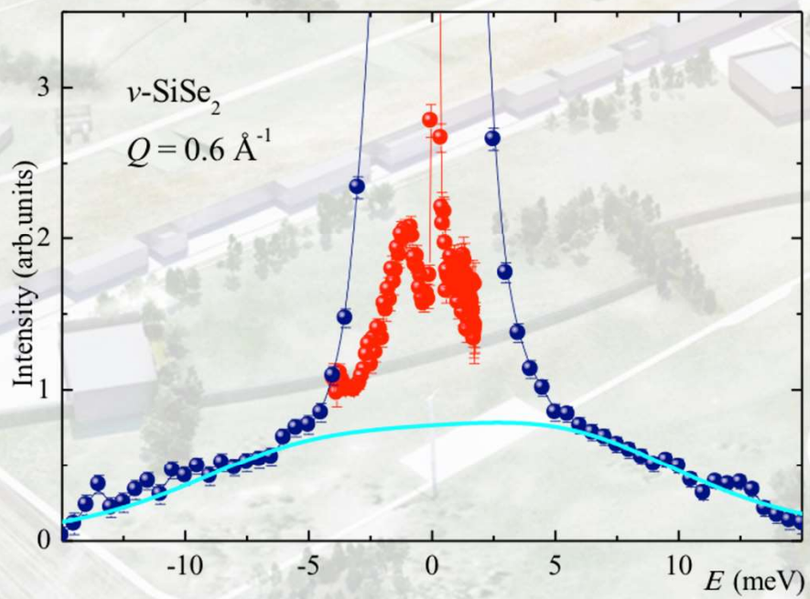
Baker et al. Nature Physics **8**, 906–911 (2012)

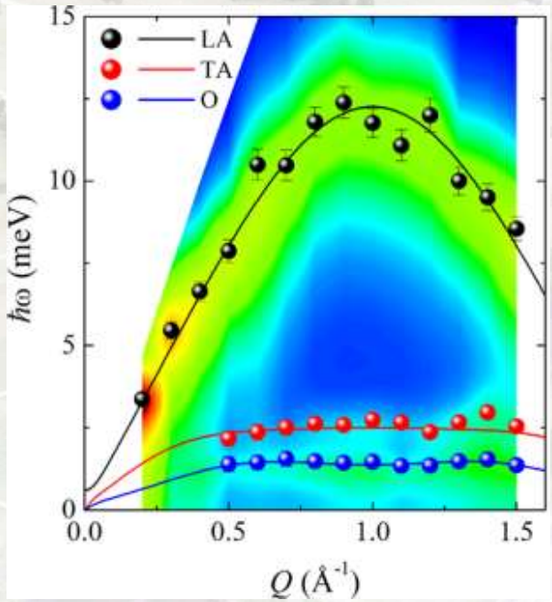
Short-wavelength collective excitations in disordered materials

- Complex multi-branched dispersion curves

(2 instruments, variable resolution)

- Multichromatic beam!

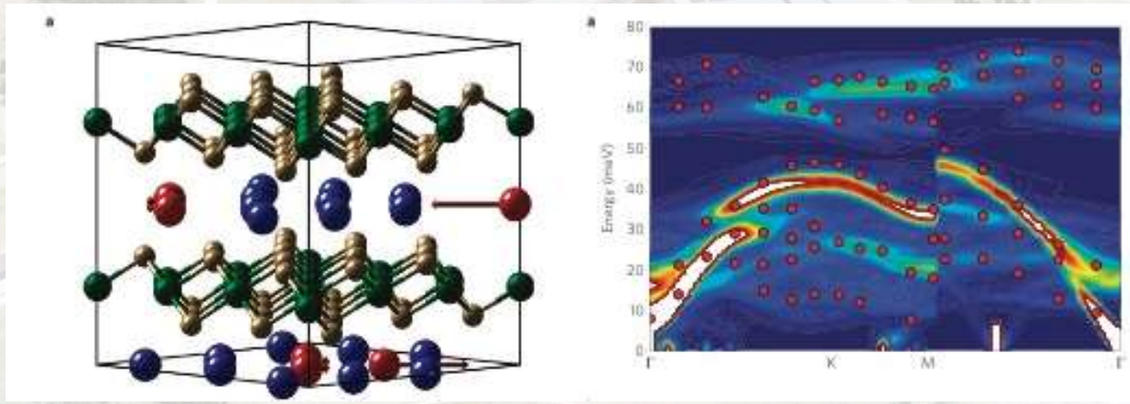




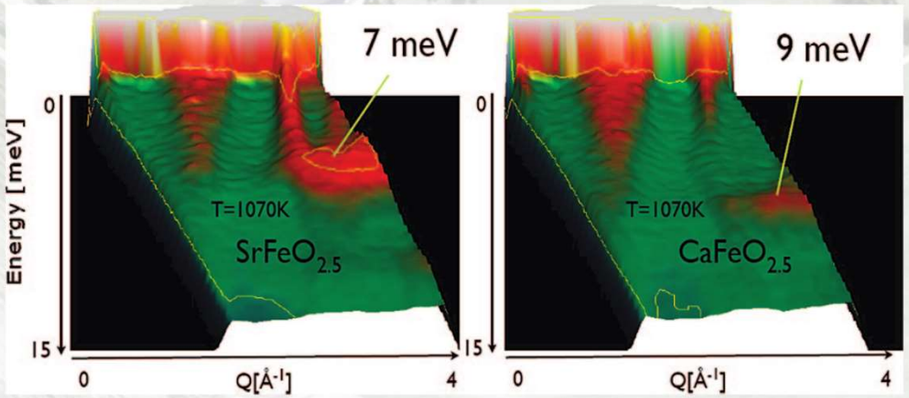
Zanatta *et al.*, J. Phys. Chem. Lett. **4**, 1143 (2013)

Materials for Energy

- Hydrogen storage
- Phonon assisted ionic conduction: from lattice dynamics to diffusive motion
  - Lattice dynamics: High excitation energy
  - Ionic Transport: tens of μeV resolution + large Q
  - Multi components: PA to separate coherent/incoherent scattering (not only H, but Li, Na, Cl,…)



Rattling in $Na_{0.8}CoO_2$
D. J. Voneshen *et al.*,
Nat. Mat. **12**, (2013) 1028



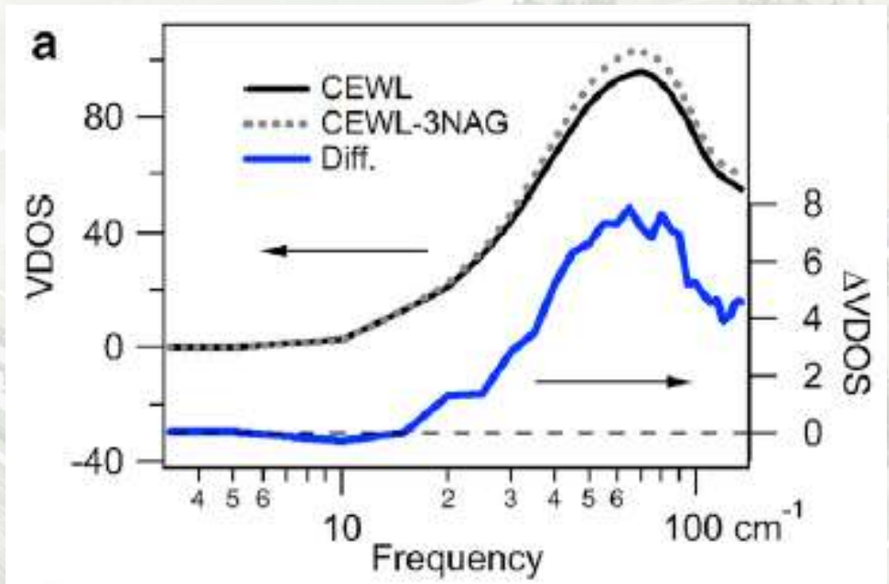
Phonon assisted oxygen mobility in SOFC
W. Paulus *et al*, JACS **130**, (2008), 16080

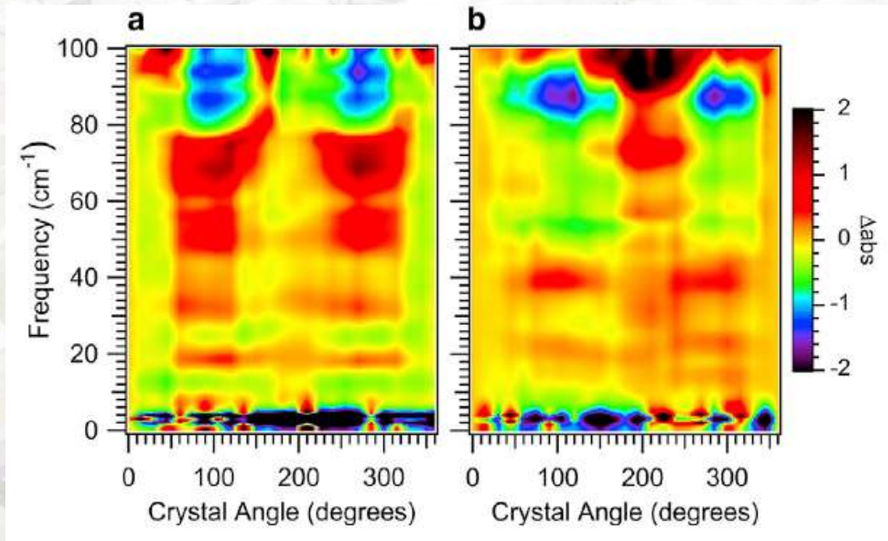
Blue-shift upon ligand binding in proteins (lysozyme)

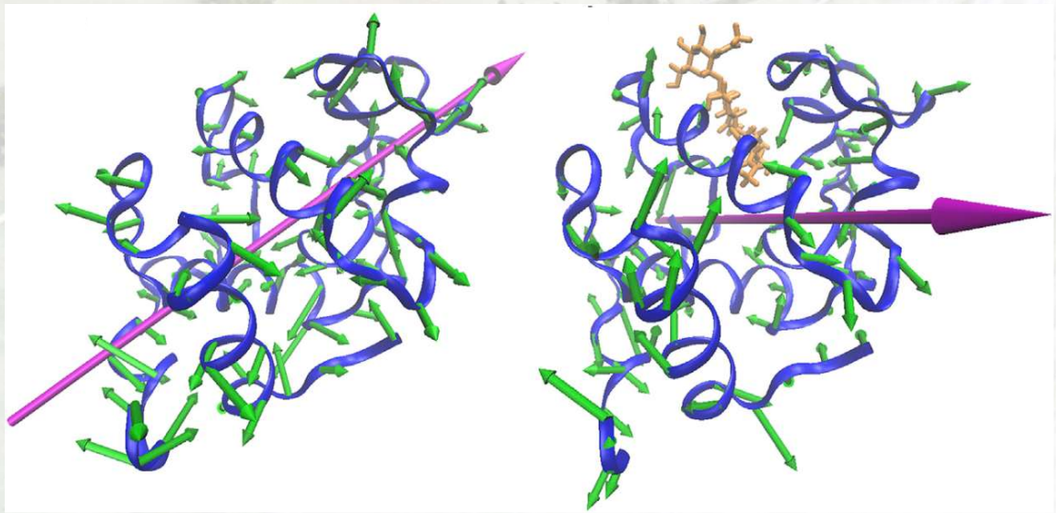
- Small and anisotropic signal from functional vibrations

(2 techniques)

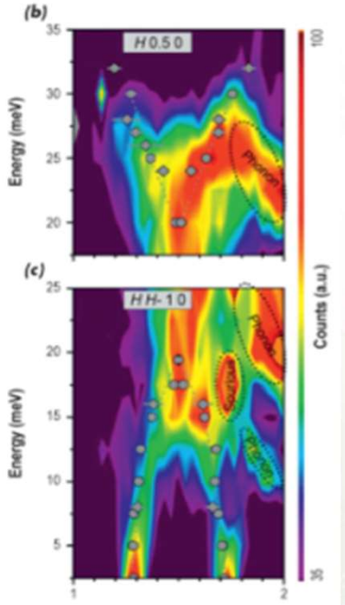
- High flux
- 4D mapping

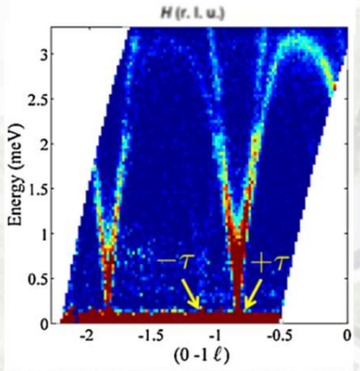


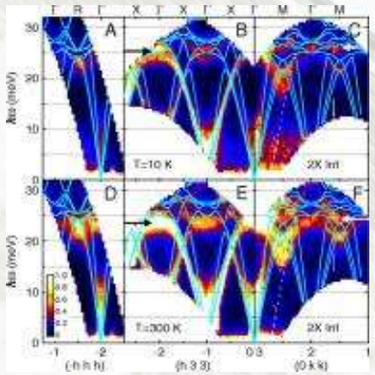




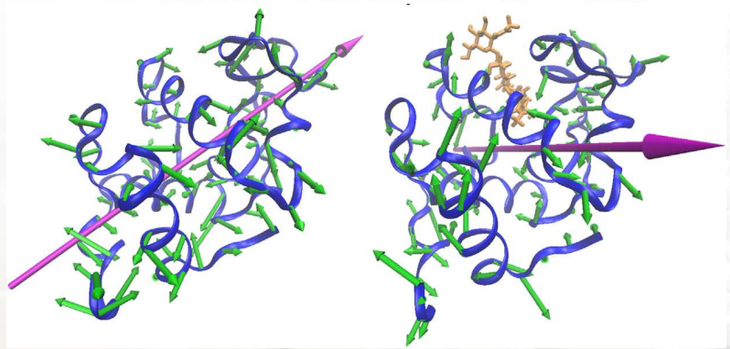
Niessen, Paciaroni, Orecchini et al., Biophys. J. 112, 933 (2017)

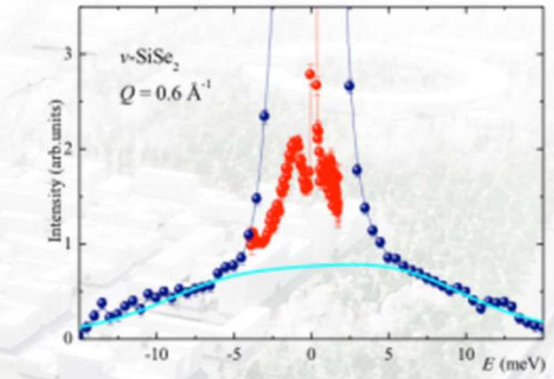


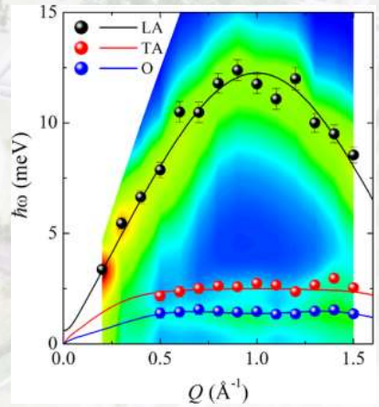


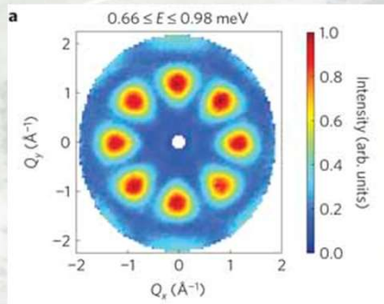


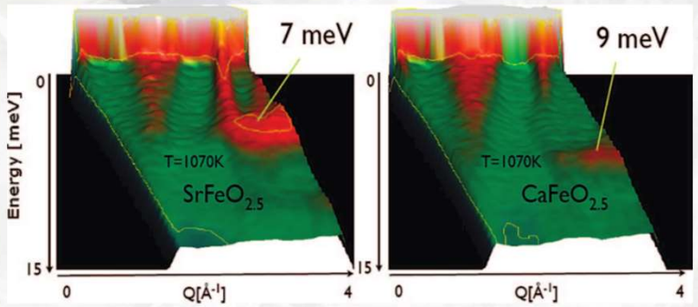
- Small signals / small samples
  (molecular magnets/nanomagnets)
- High-flux / high resolution
- Wide 4D dynamic range
- Polarization Analysis
  (magnetism + separation of coherent and spin-incoherent signals)
- “Smart” sample environment
  (pump & probe/strobo)











T-REX
Time-of-flight Reciprocal space Explorer

A neutron spectrometer for

magnetism,

material science,

soft matter

at ESS

Thank you!