Wide-angle polarization analysis at ISIS: past, present, and future

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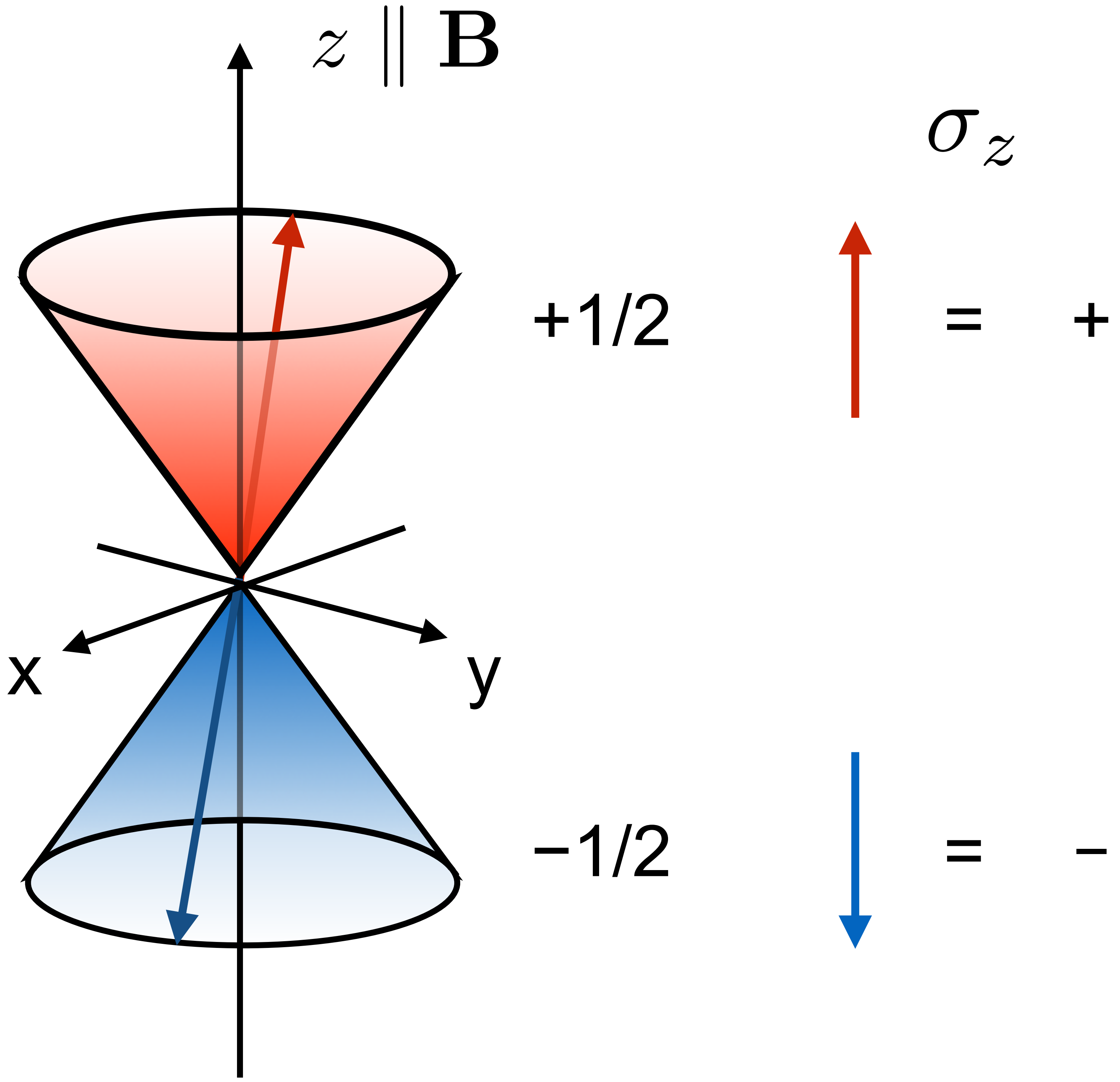
Science and Technology Facilities Council

ICANS 01/11/2023

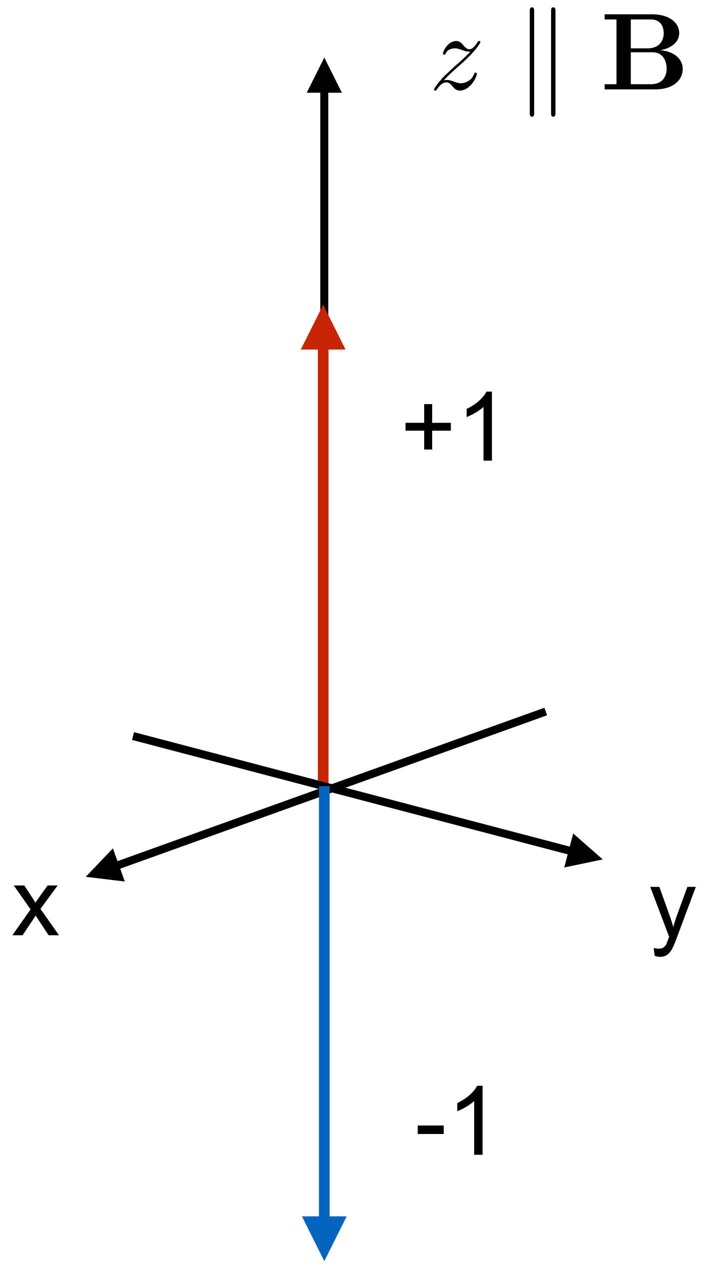
What is a polarized beam?

- Neutrons are S = 1/2 particles, and therefore have a magnetic moment:

Single neutron



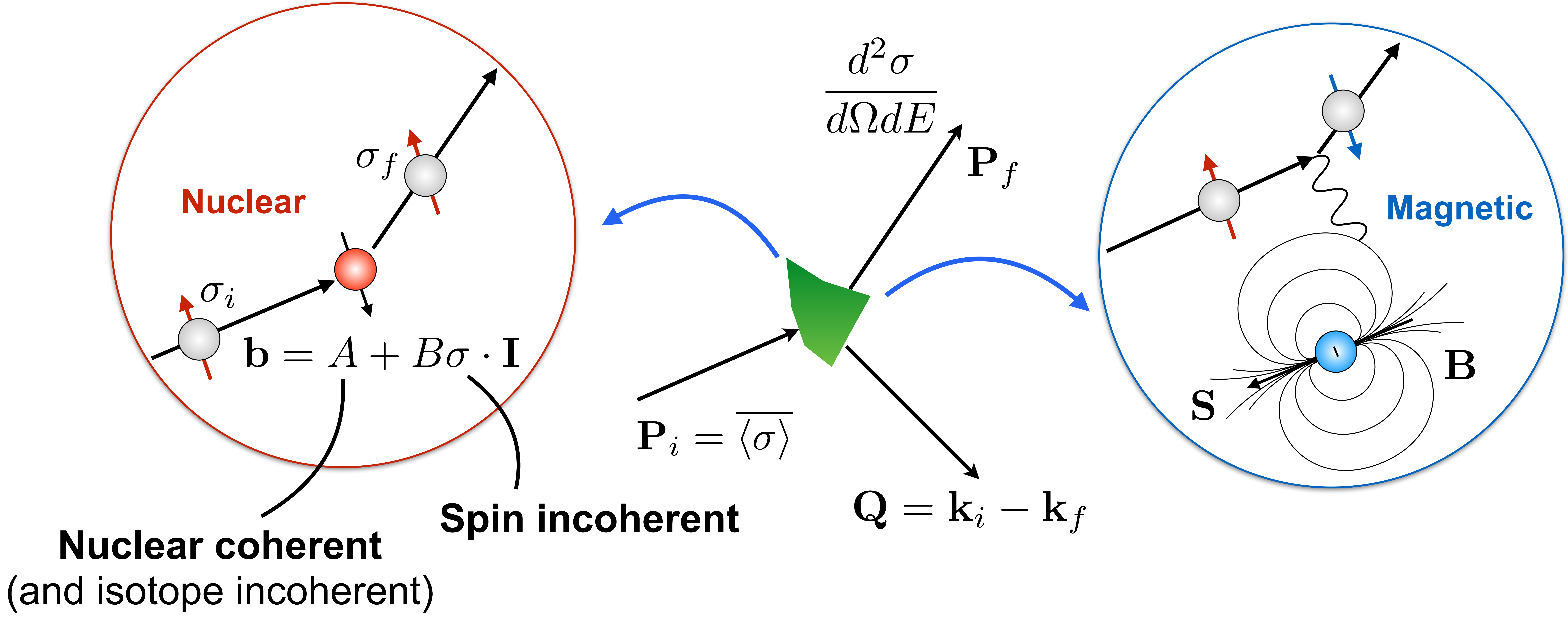
Beam of neutrons



$$\mathbf{P} = \overline{\langle \sigma \rangle} = (0, 0, P_z)$$

$$P_z = \frac{N_+^z - N_-^z}{N_+^z + N_-^z}$$

Why polarized neutrons?



Why polarized neutrons?

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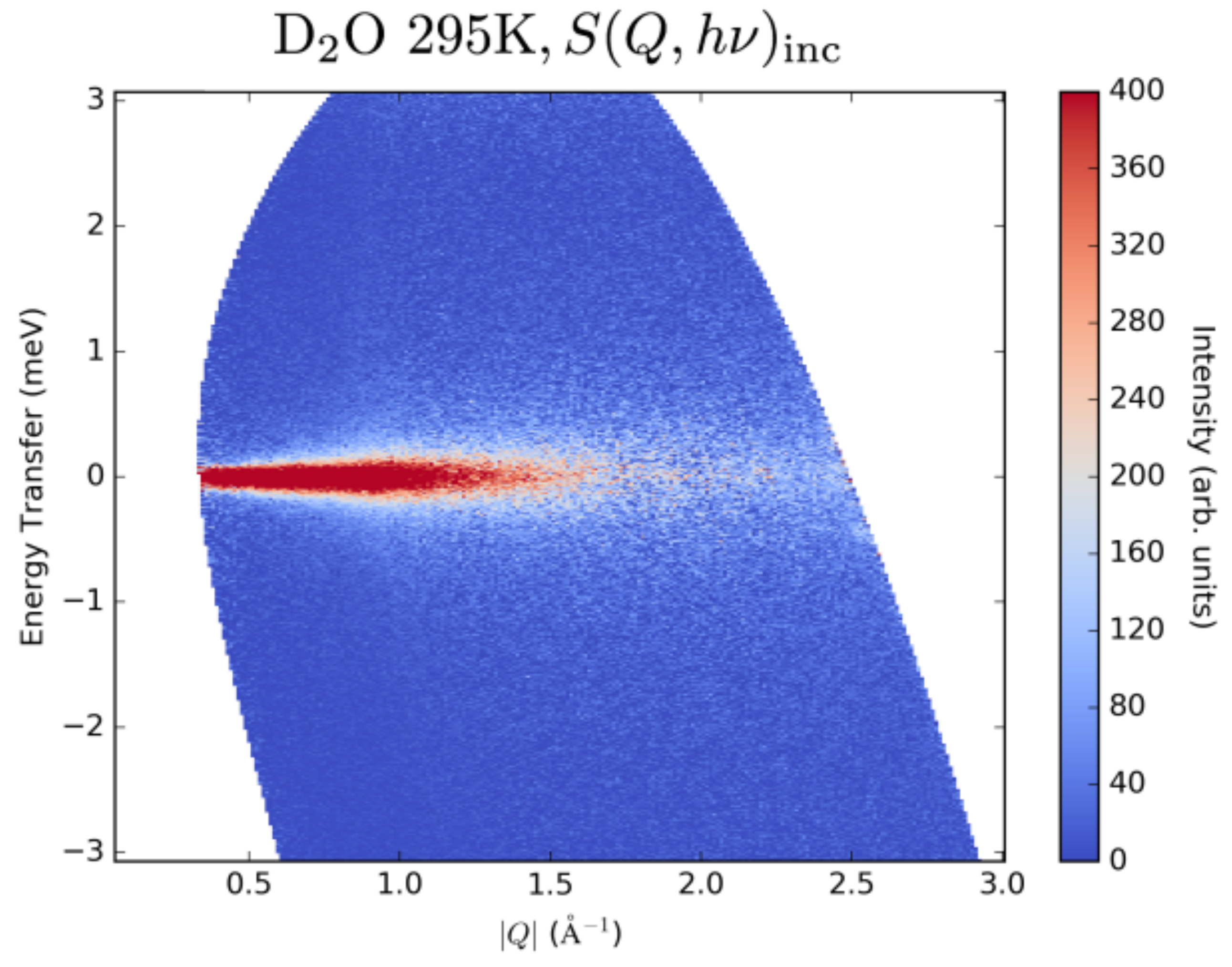
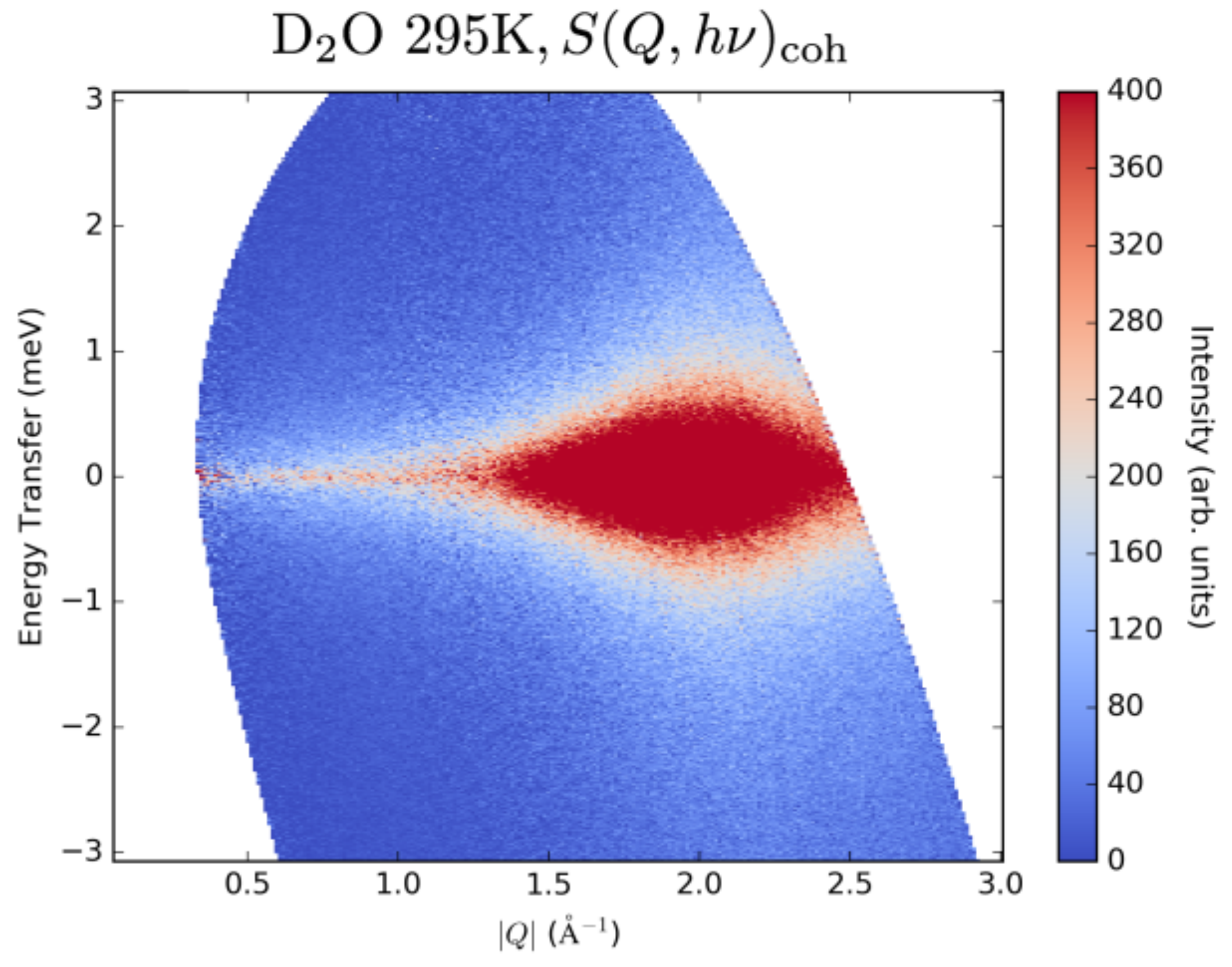
- Extra information on cross section components and moment direction:

Component Separation

Spin incoherent
Self-correlations

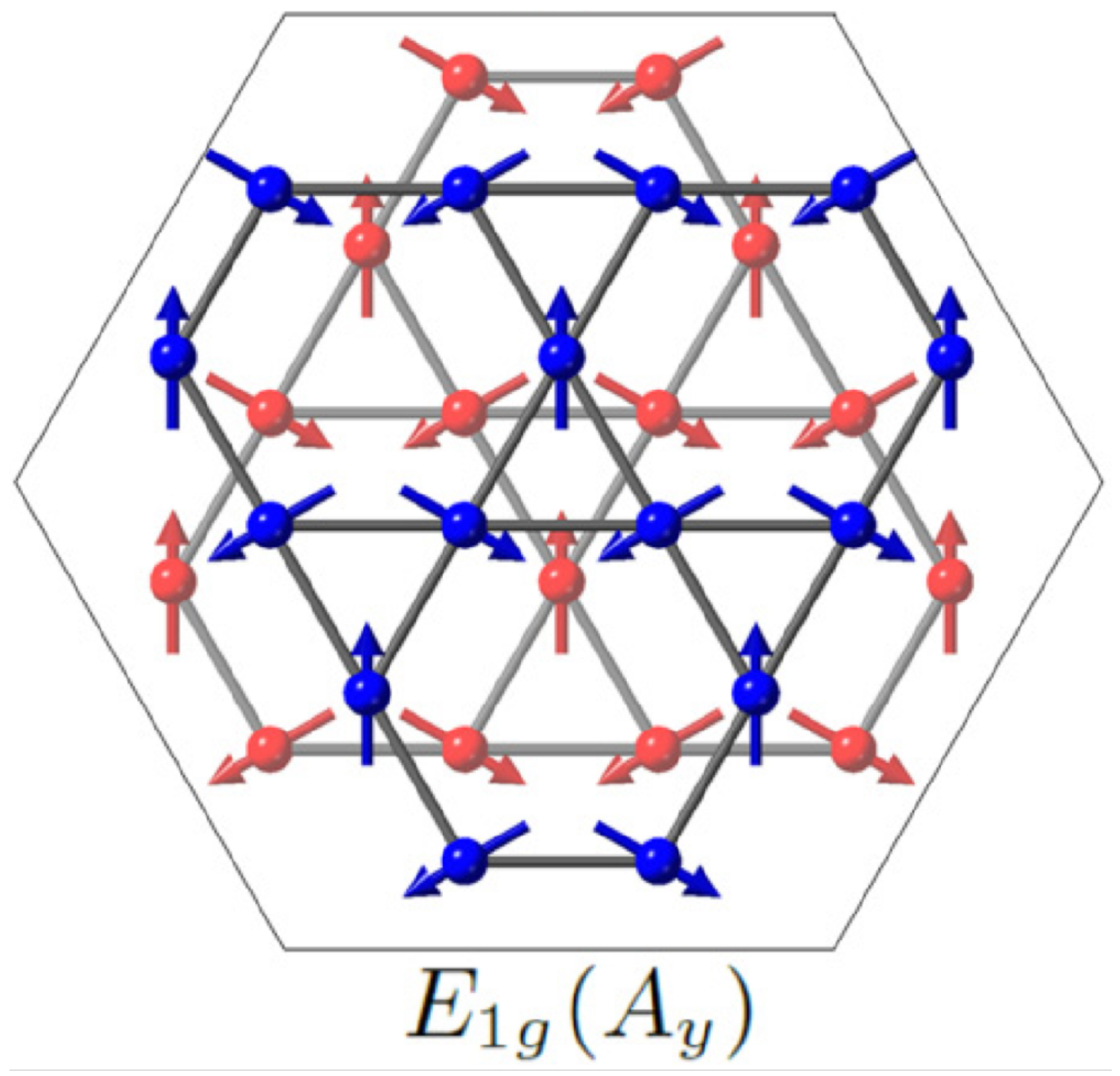


Coherent
Self and collective corr.



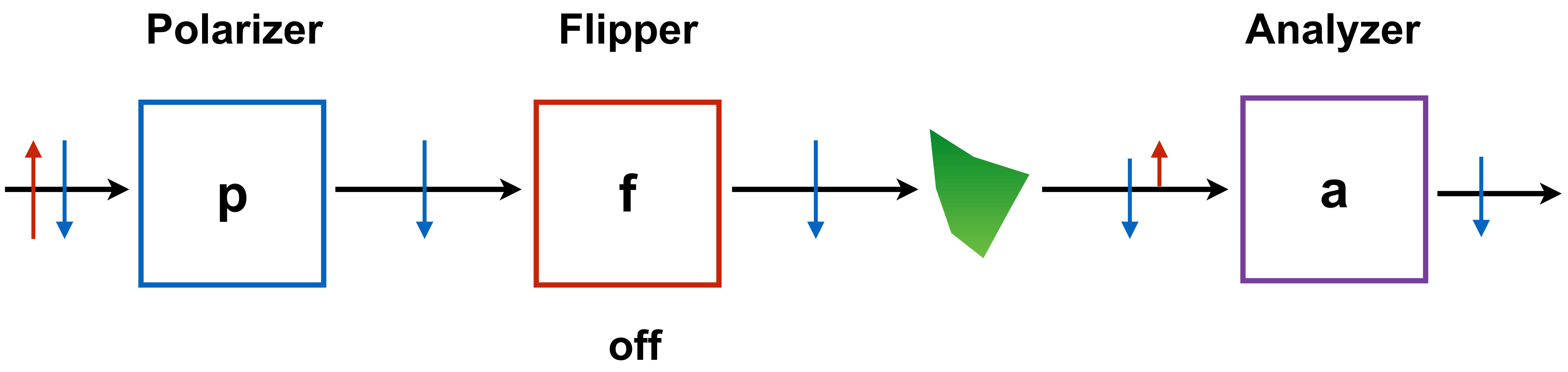
Arbe et. al., Phys. Rev. Research **2**, 022015(R) (2020)

Complex Magnetism



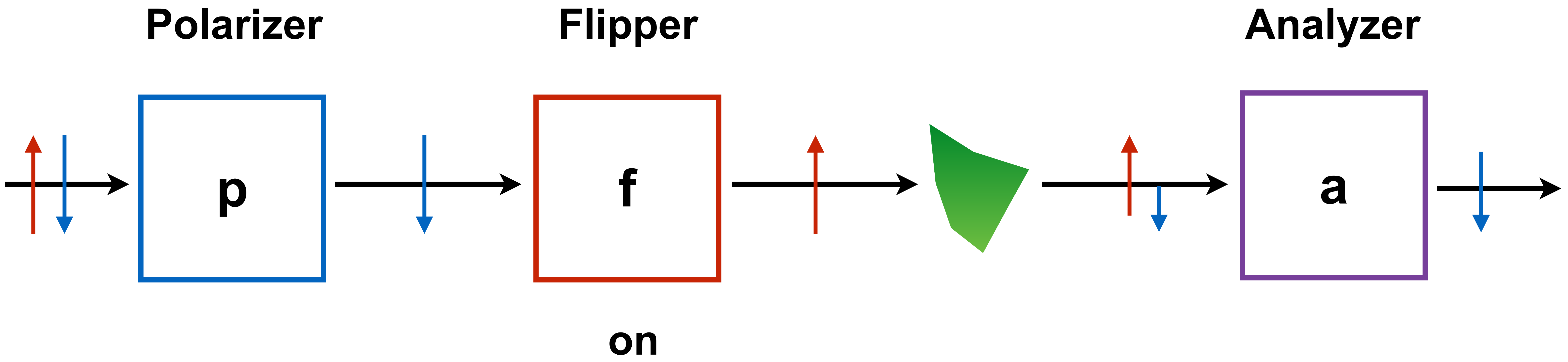
Soh *et al.*, PRB **101**, 140411 (2020)

Longitudinal polarization analysis



	Coherent	Spin incoherent	Paramagnetic powder	Magnetic crystal
Non spin flip	1	1/3	$\frac{1}{2}\left[1-(\hat{\mathbf{P}}\cdot\hat{\mathbf{Q}})^2\right]$	$[\hat{Q}\times M(\mathbf{Q})\times\hat{Q}]_{\|\|\mathbf{P}}$
Spin flip	0	2/3	$\frac{1}{2}\left[1+(\hat{\mathbf{P}}\cdot\hat{\mathbf{Q}})^2\right]$	$[\hat{Q}\times M(\mathbf{Q})\times\hat{Q}]_{\perp\mathbf{P}}$

Longitudinal polarization analysis



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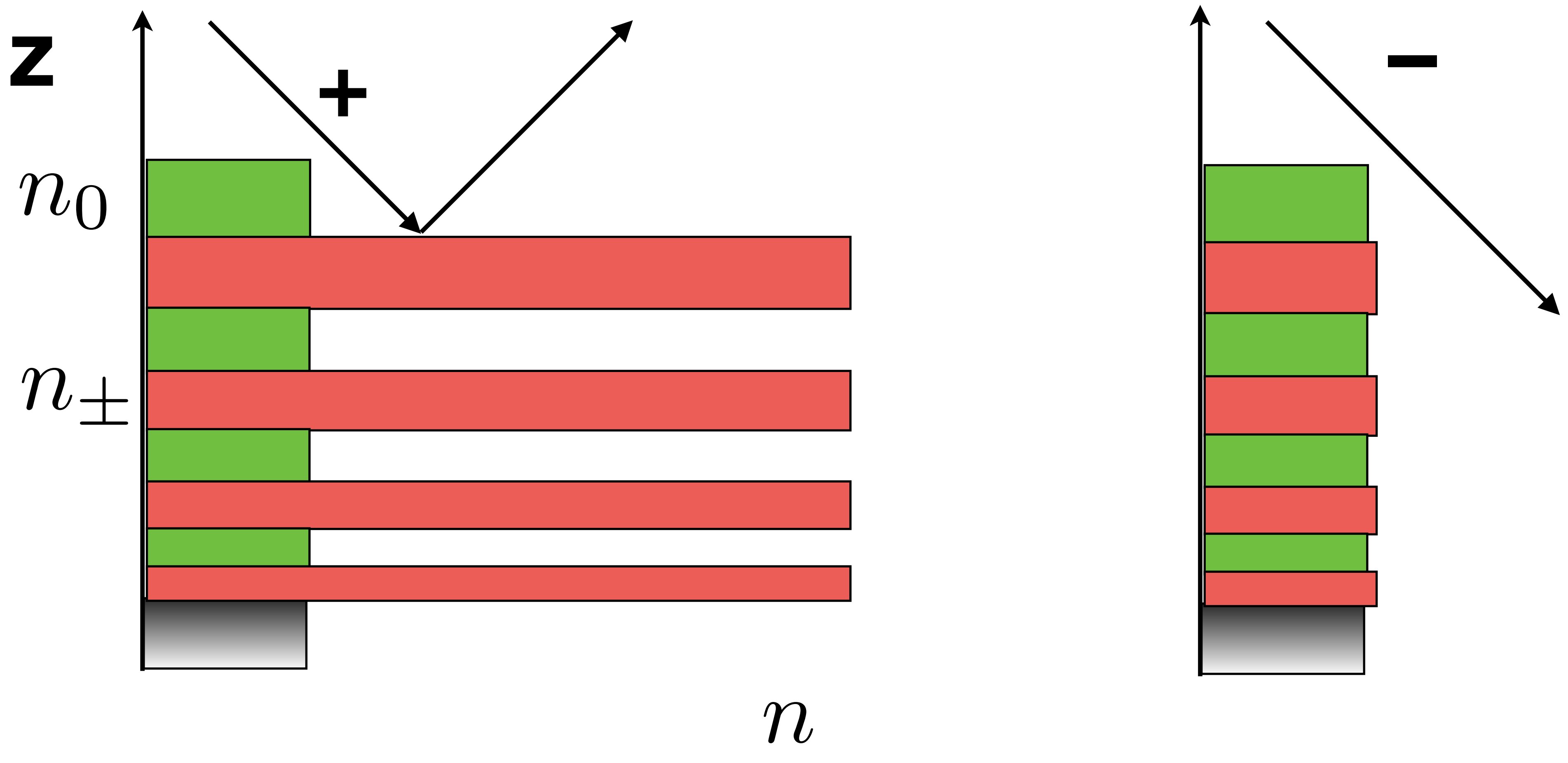
How to polarize and analyse neutrons?

- There are three main ways of polarising or analysing a neutron beam: polarising crystals, ^{3}He spin filters, and supermirrors:

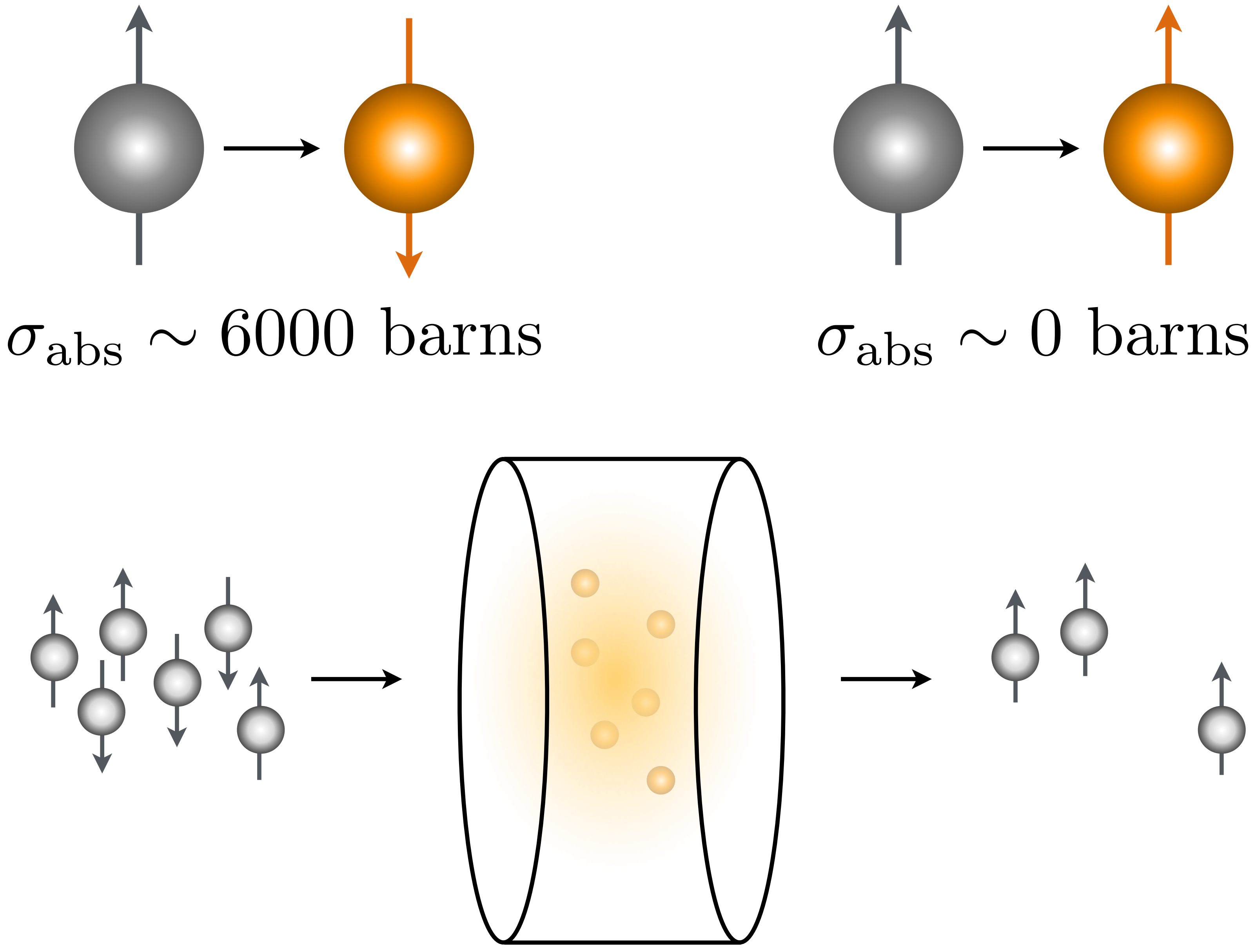
Supermirror

$$n_\pm \propto \sqrt{\rho_{\mathrm{coh}} \mp \rho_{\mathrm{mag}}}$$



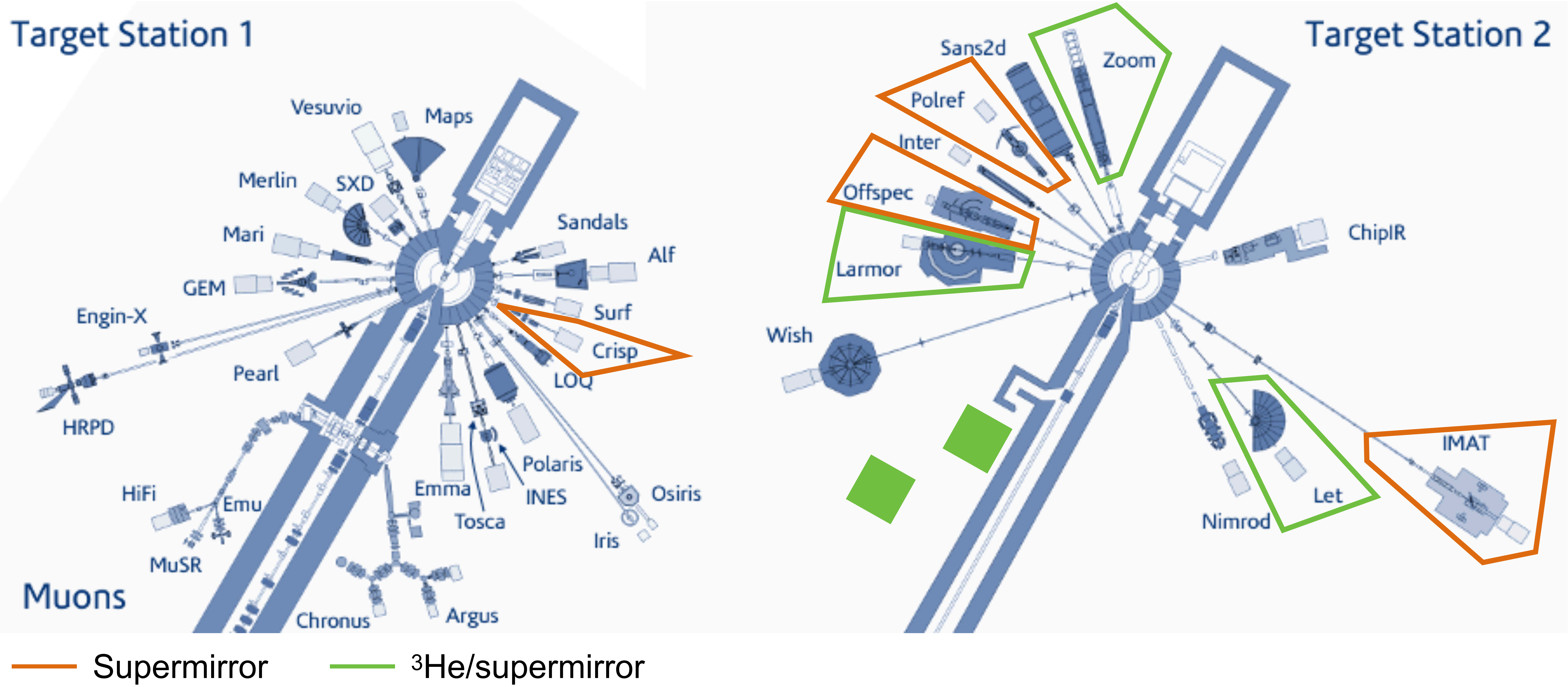
$$R = \left(\frac{n_0 - n_\pm}{n_0 + n_\pm}\right)^2$$

^{3}He spin filter



Polarized neutrons at ISIS

- Zoom, Larmor (SANS/SE), LET (DTOF), Offspec, Polref (refl.) IMAT (imaging)



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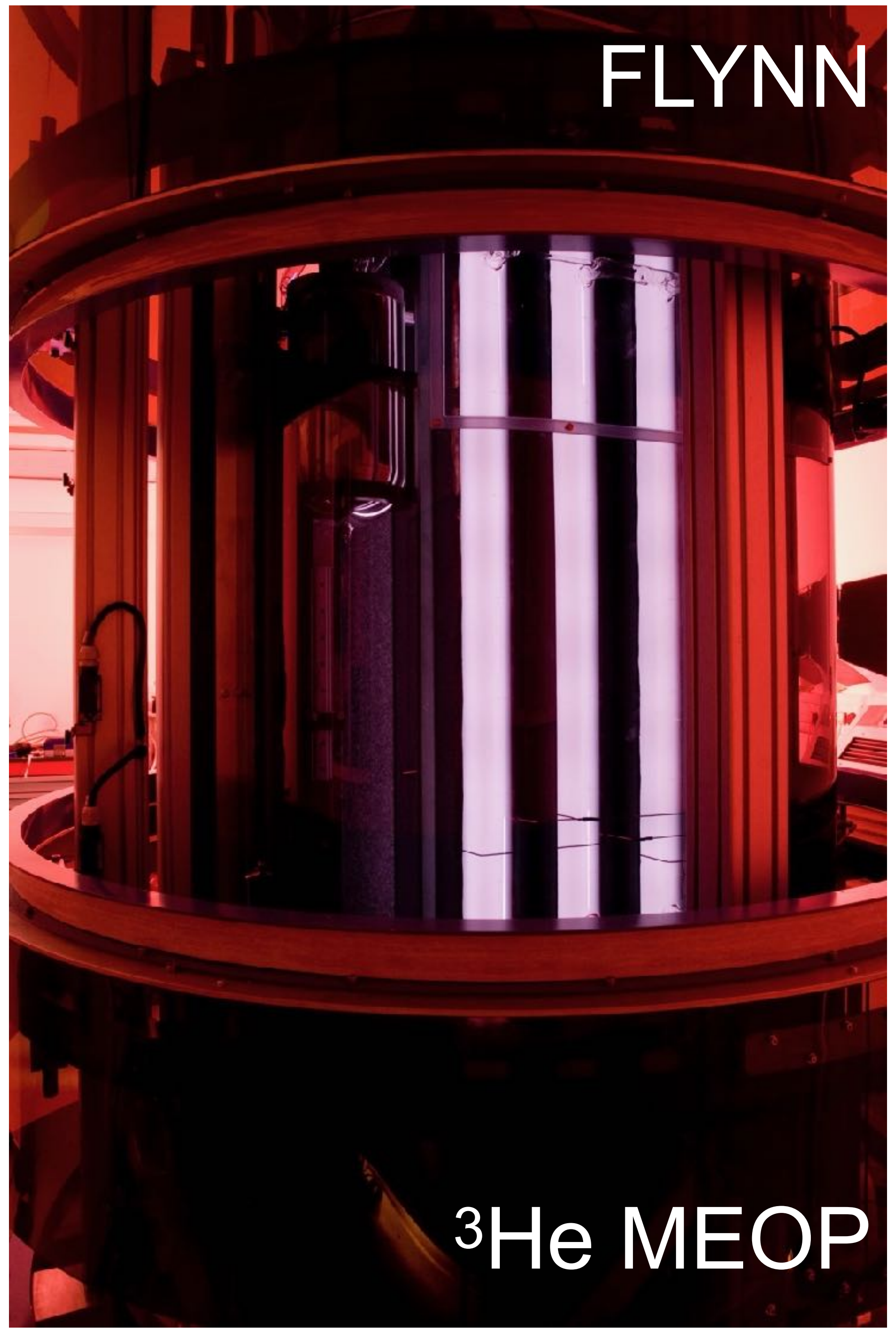

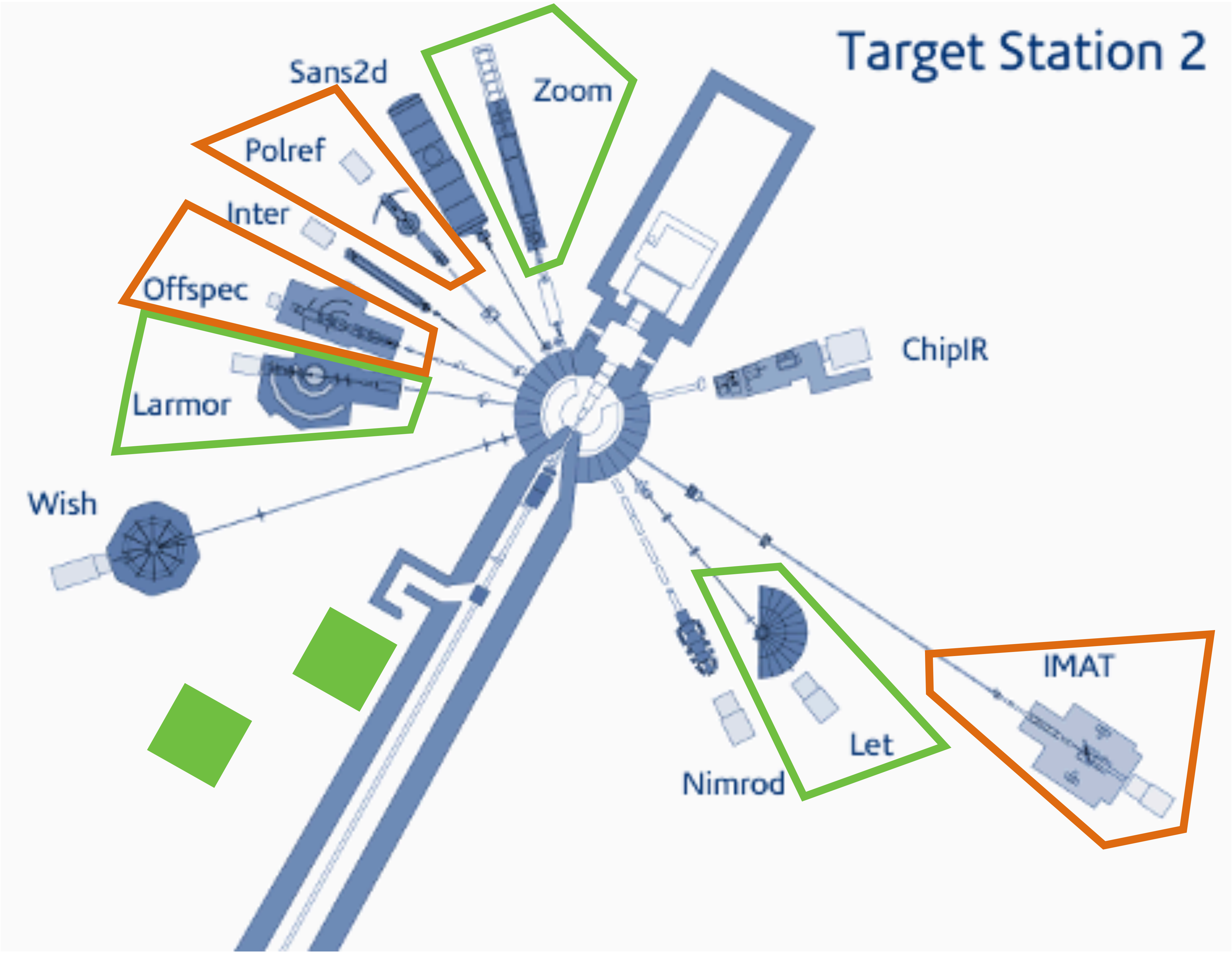

Supermirror ^{3}He/supermirror

Wide-angle polarization analysis at ISIS

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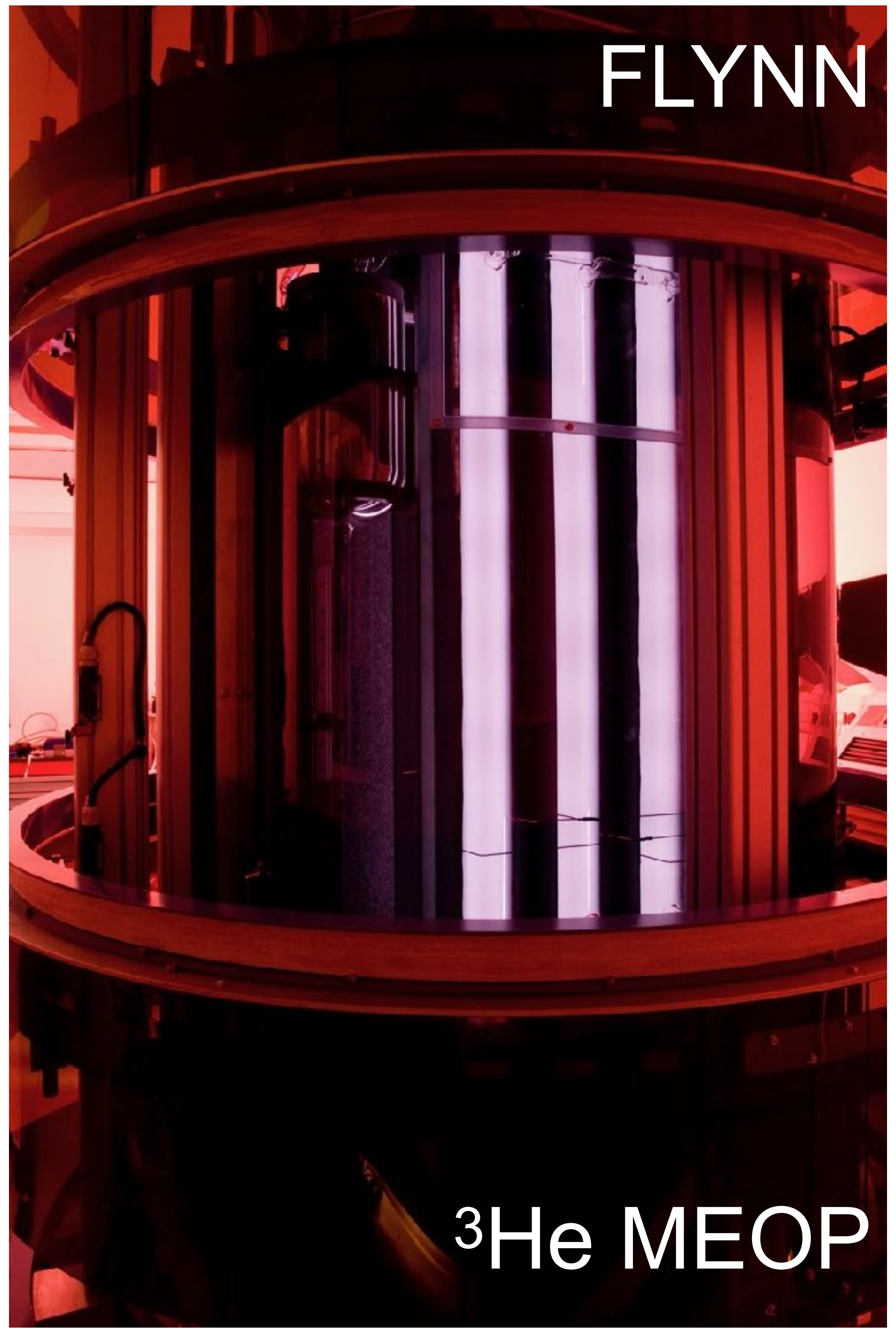
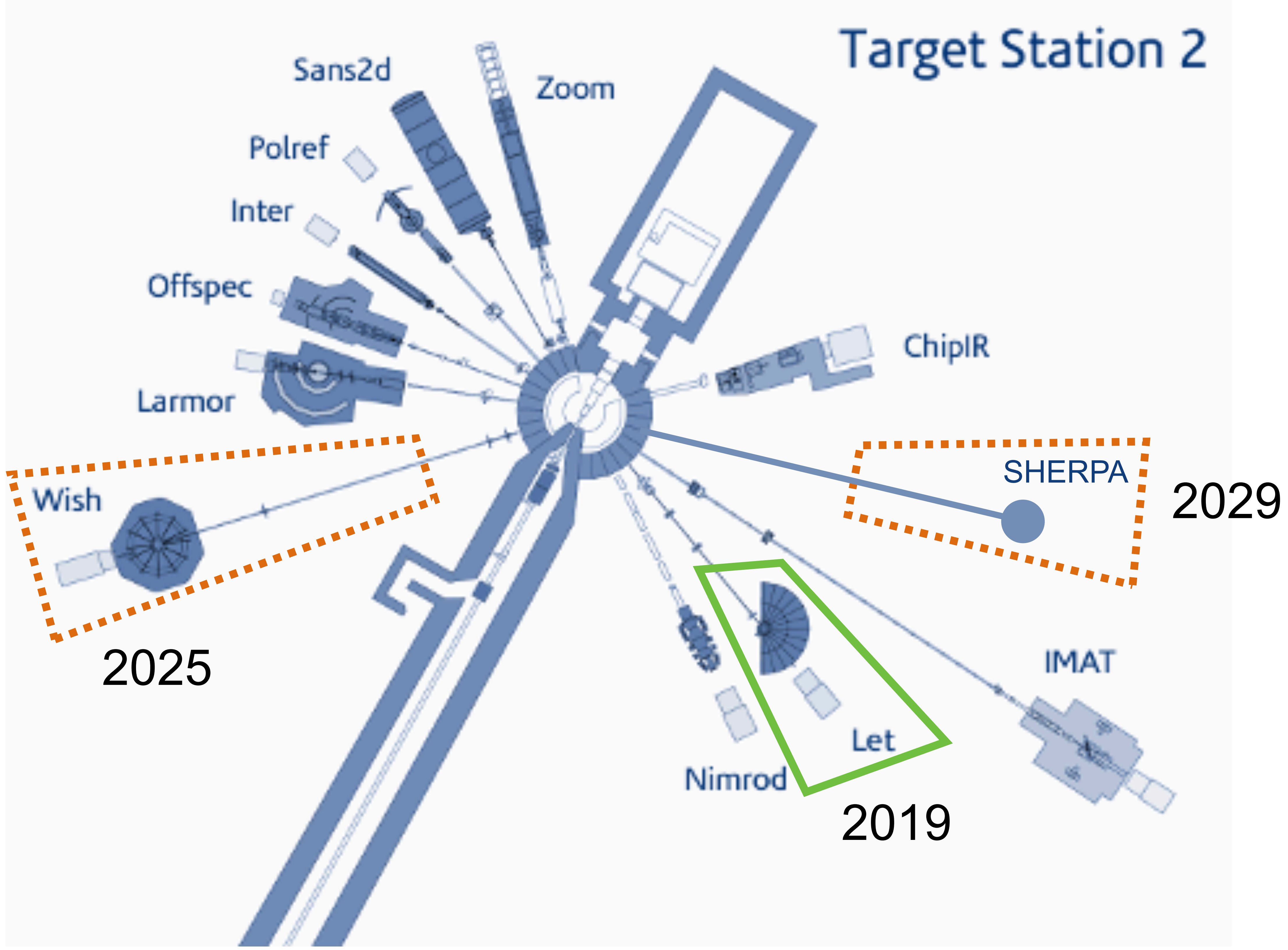
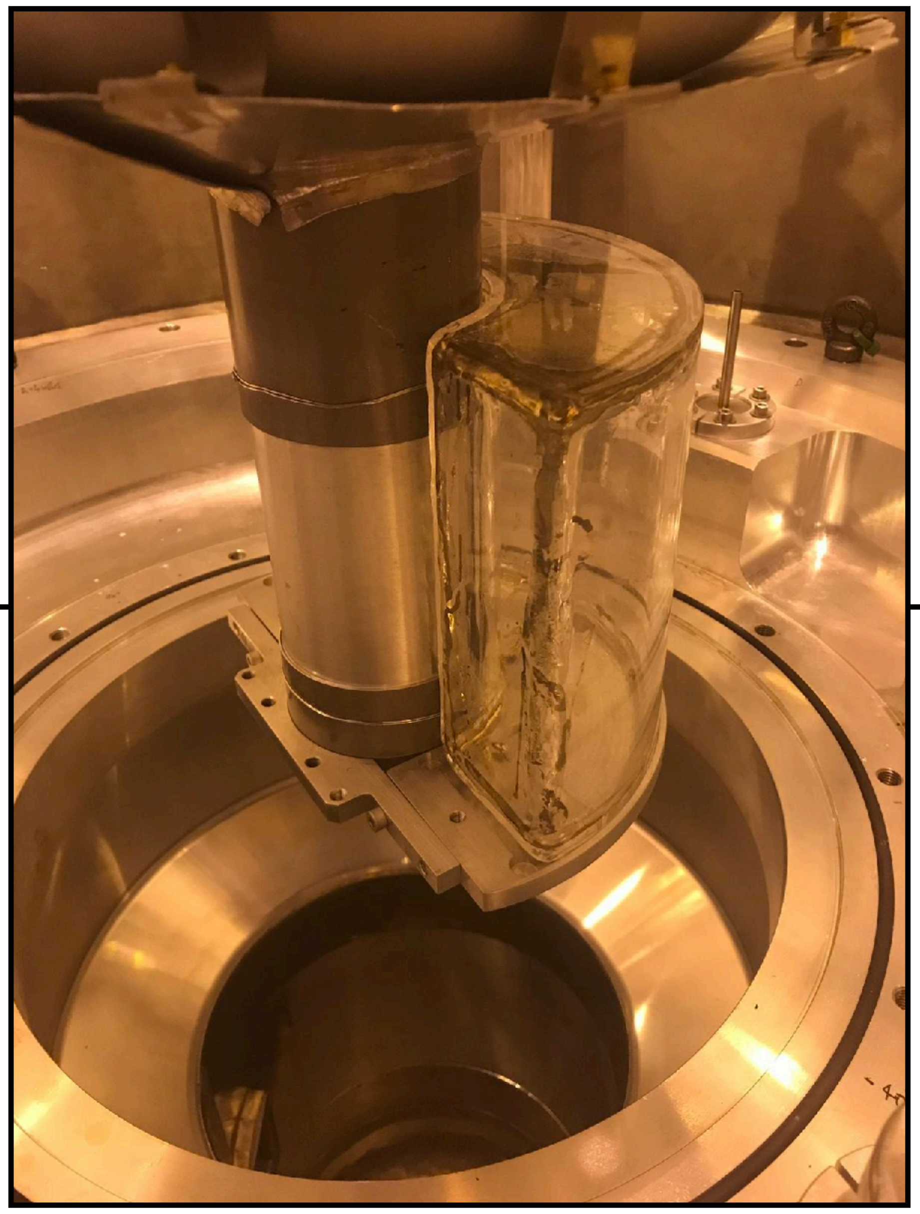
- LET (DTOF), WISH (diffraction), SHERPA (ITOF)



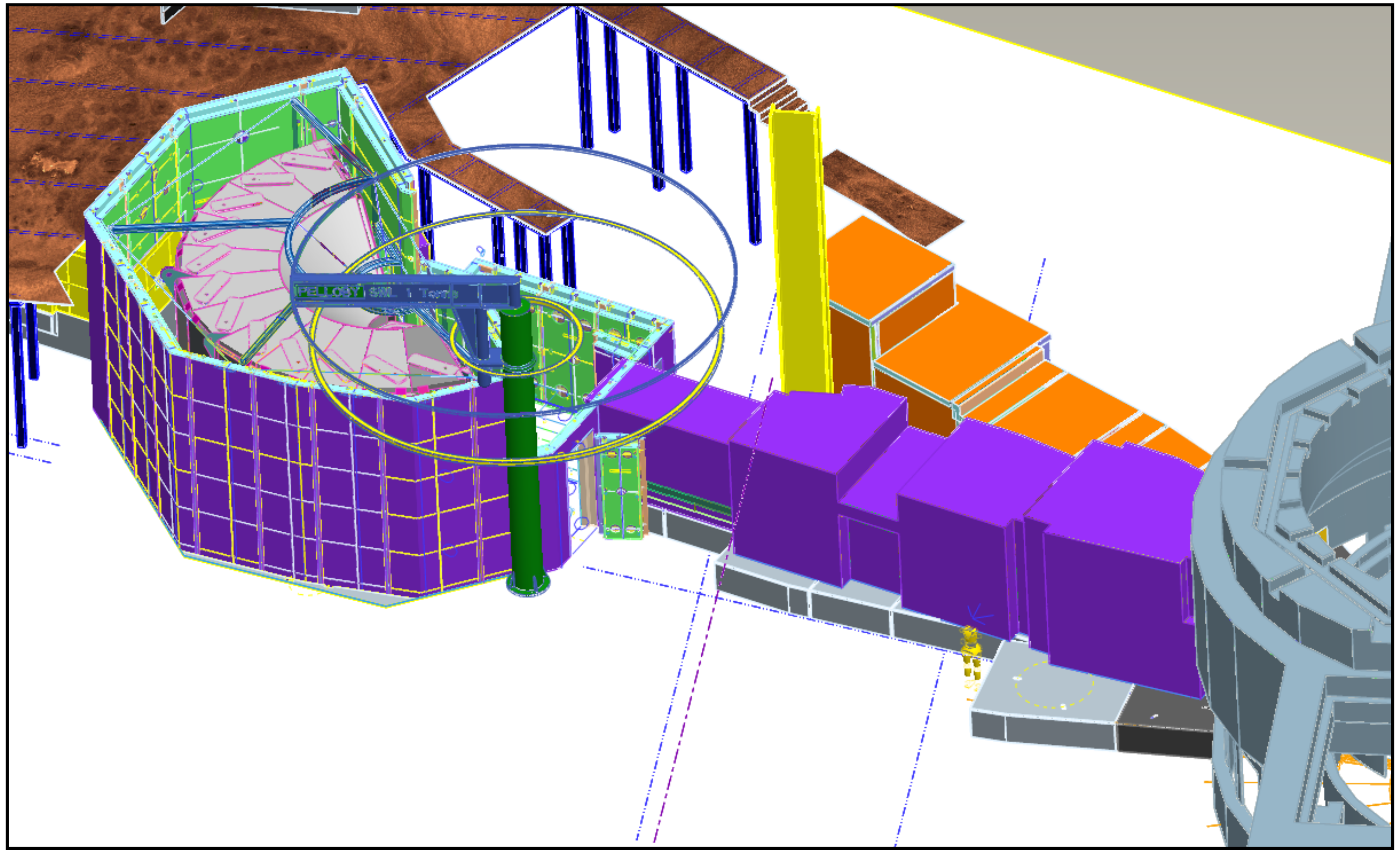


Supermirror — ^{3}He/supermirror

Past: Polarization analysis on LET



The LET spectrometer



E_i 1 - 25 meV

Resolution 1 - 4 %

ϕ (3 Å) 3 x 10^5 $ncm^{-2}s^{-1}$

Beam size 2 x 4 cm^2

Detectors ^3He PSD

Coverage π st.

“Cathedral” of neutron scattering

Science on LET: 2017

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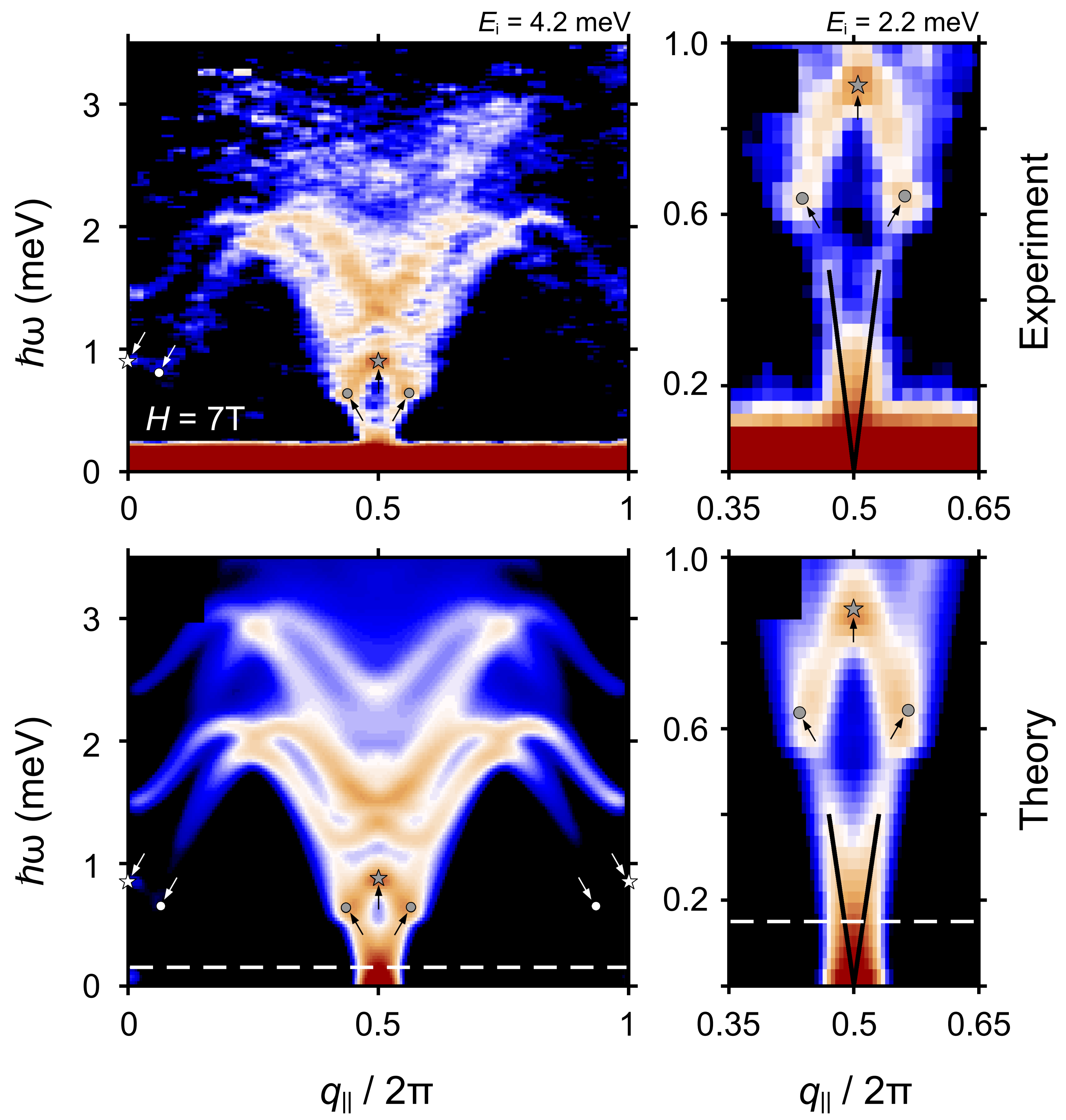
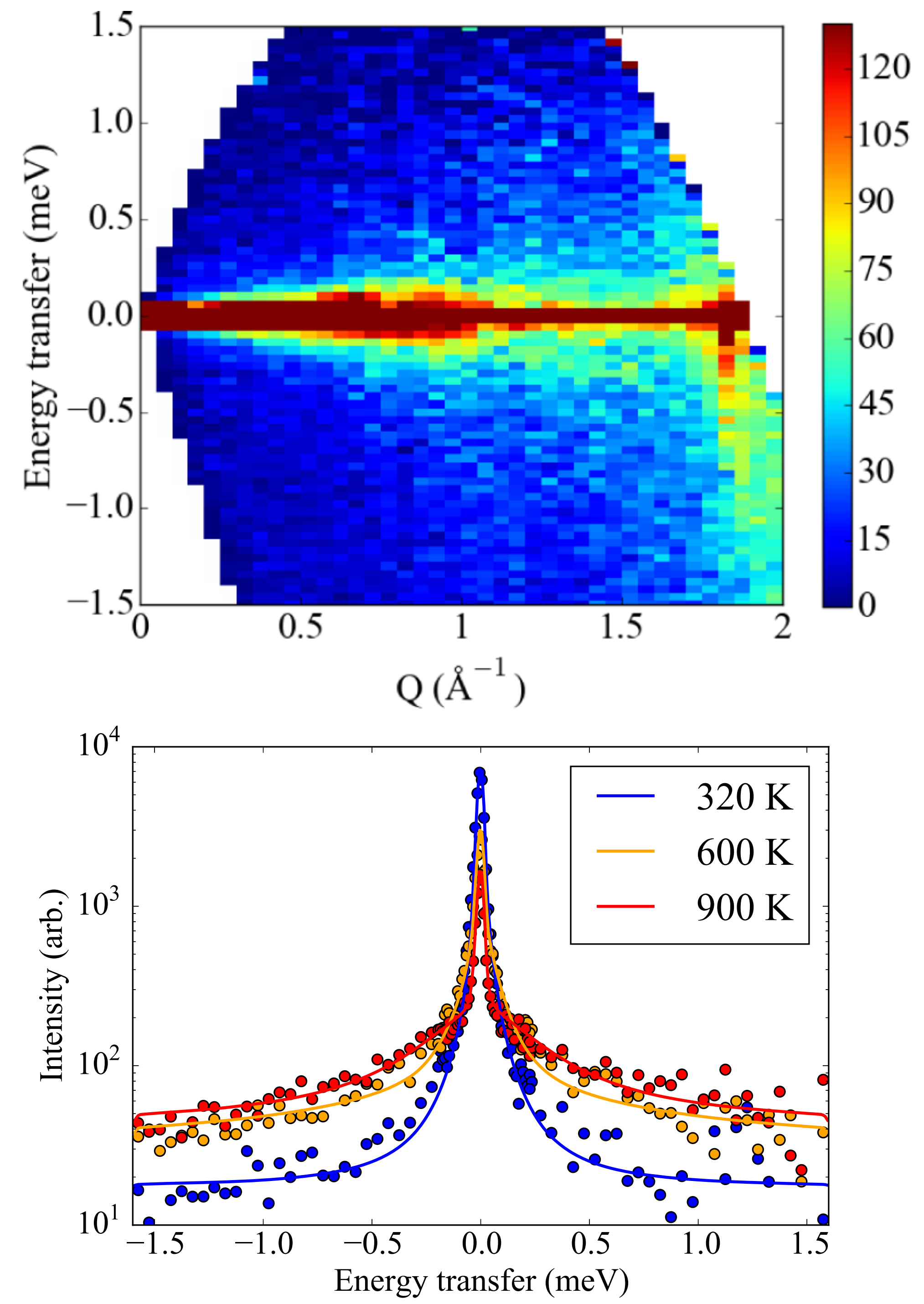
Magnetism (80%)



e.g. exotic phases in quantum magnets

Schmidiger et. al. PRL **115** 147201

QENS (20%)



e.g. diffusion in ionic conductors

Voneshen et. al. PRL **118** 145901

Incoherent/coherent separation

- Polarized neutrons allow us to distinguish **incoherent** (single-particle motions) from **coherent** (collective and single-particle motions)

	σ_{coh} (barn)	σ_{inc} (barn)
H	1.7583	80.27
^{7}Li	0.619	0.78
Na	1.66	1.62
D	5.592	2.05
Cu	7.485	0.55
O	4.232	0.008

dominant incoherent

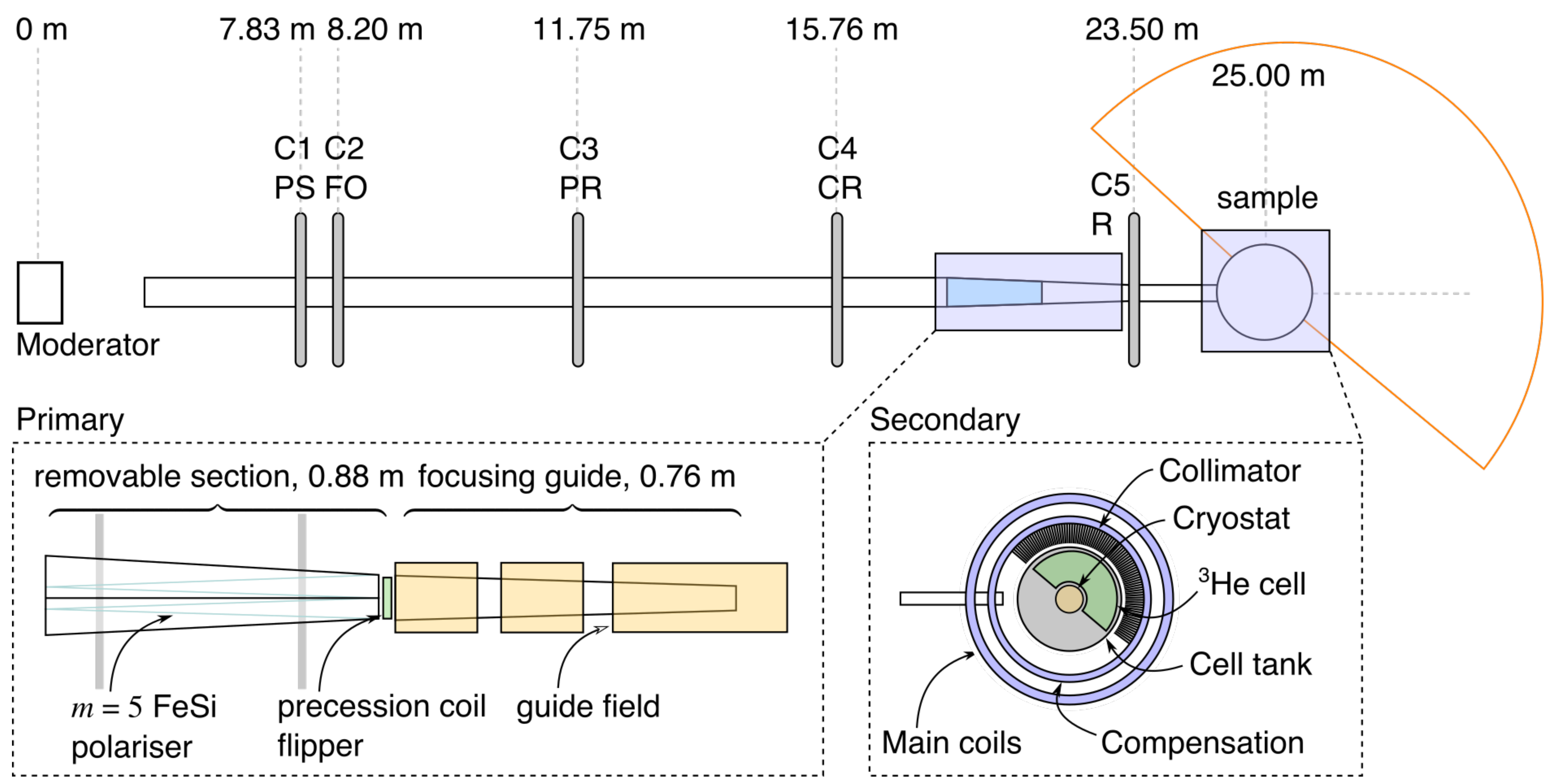
↓

difficult to distinguish

↓

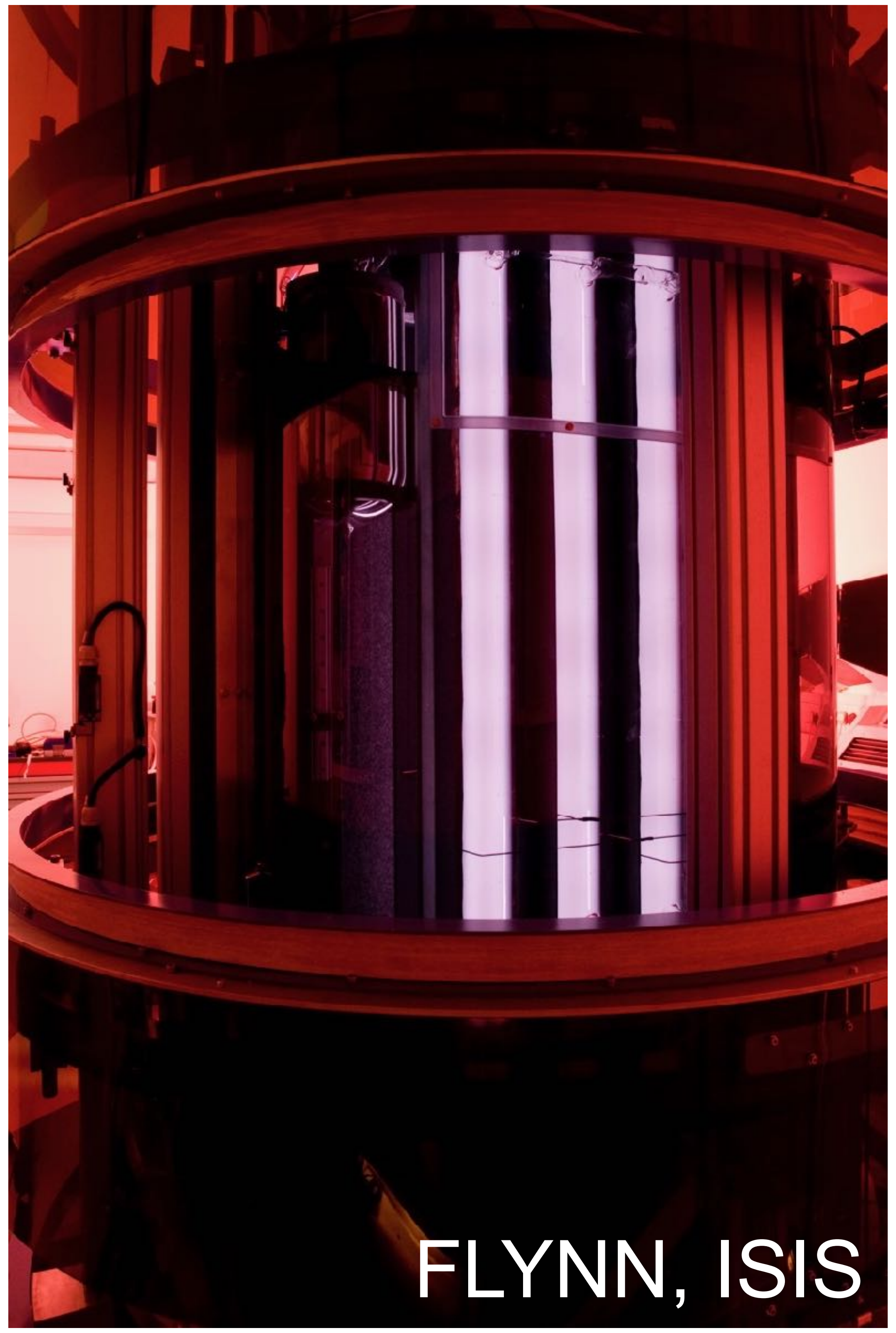
dominant coherent

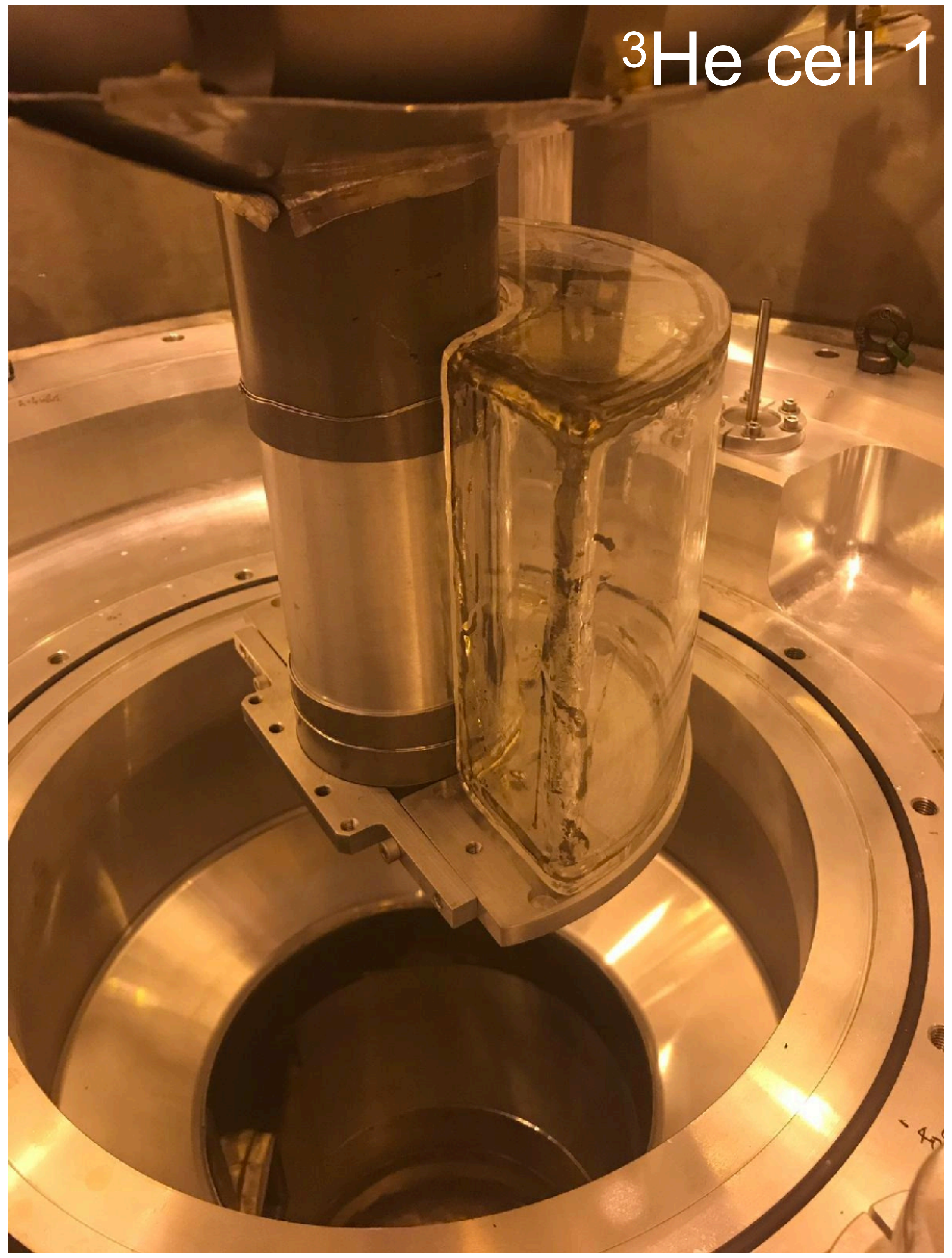
Instrument layout



Nilsen et. al. J. Phys.: Conf. Series **115** 012019

Implementation: analyzer

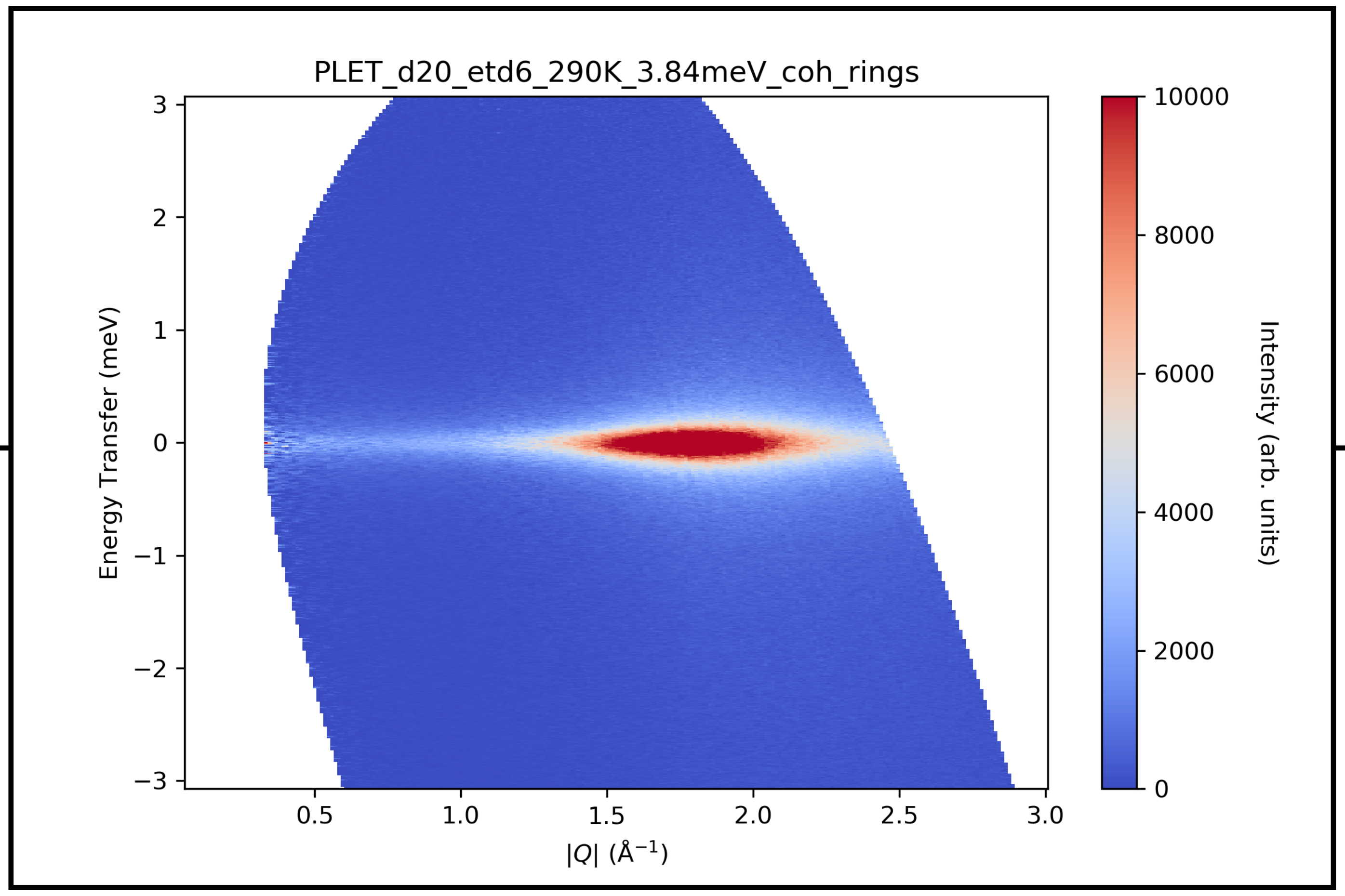




P_0 ~ 65 %

T_1 = 100 hours

Cell change: ~30s



Present: LET Science Examples

Science on LET: current

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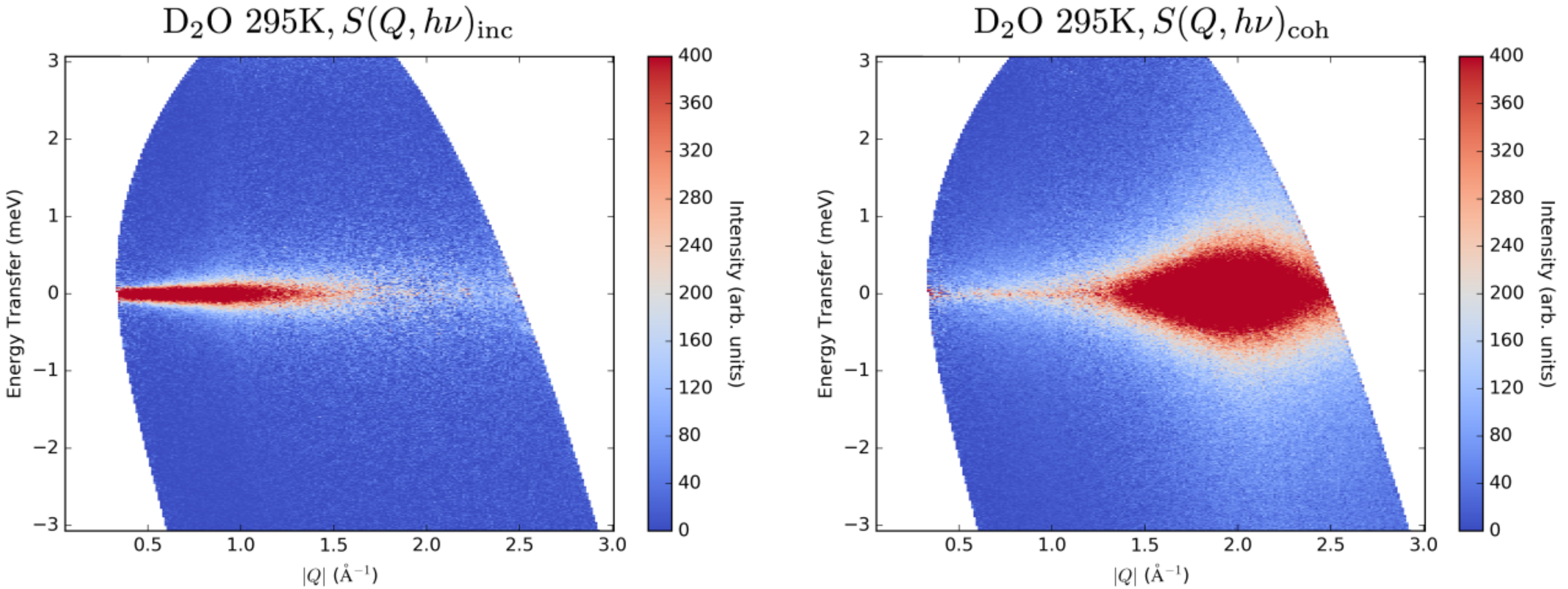
QENS (30% - 15% polarized)



Arbe et. al., Phys. Rev. Research **2**, 022015(R) (2020)

Diffusion in solvent mixtures



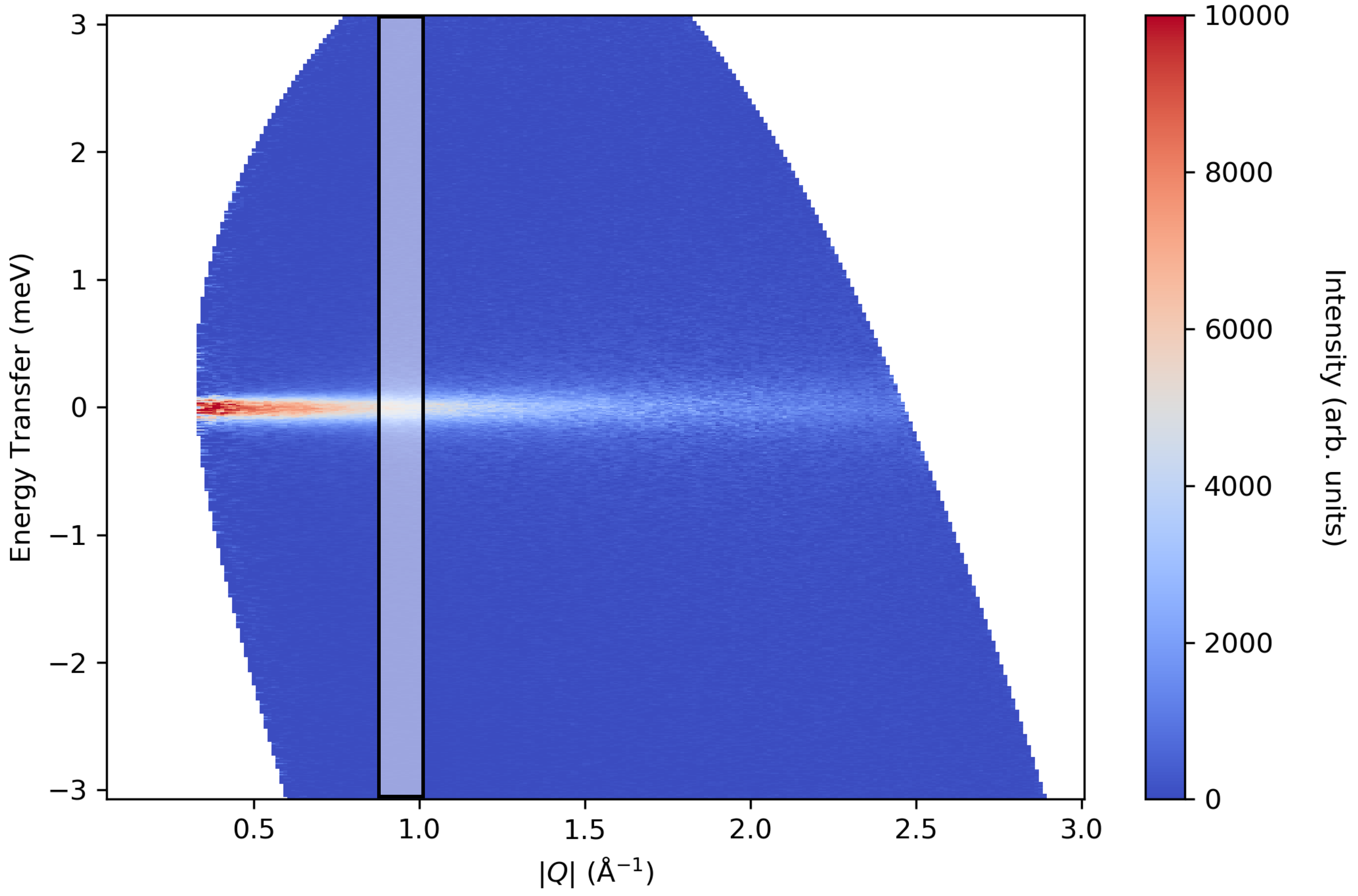


K. Edkins R. Morbidini R. Edkins K. Nemkovski T. Seydel

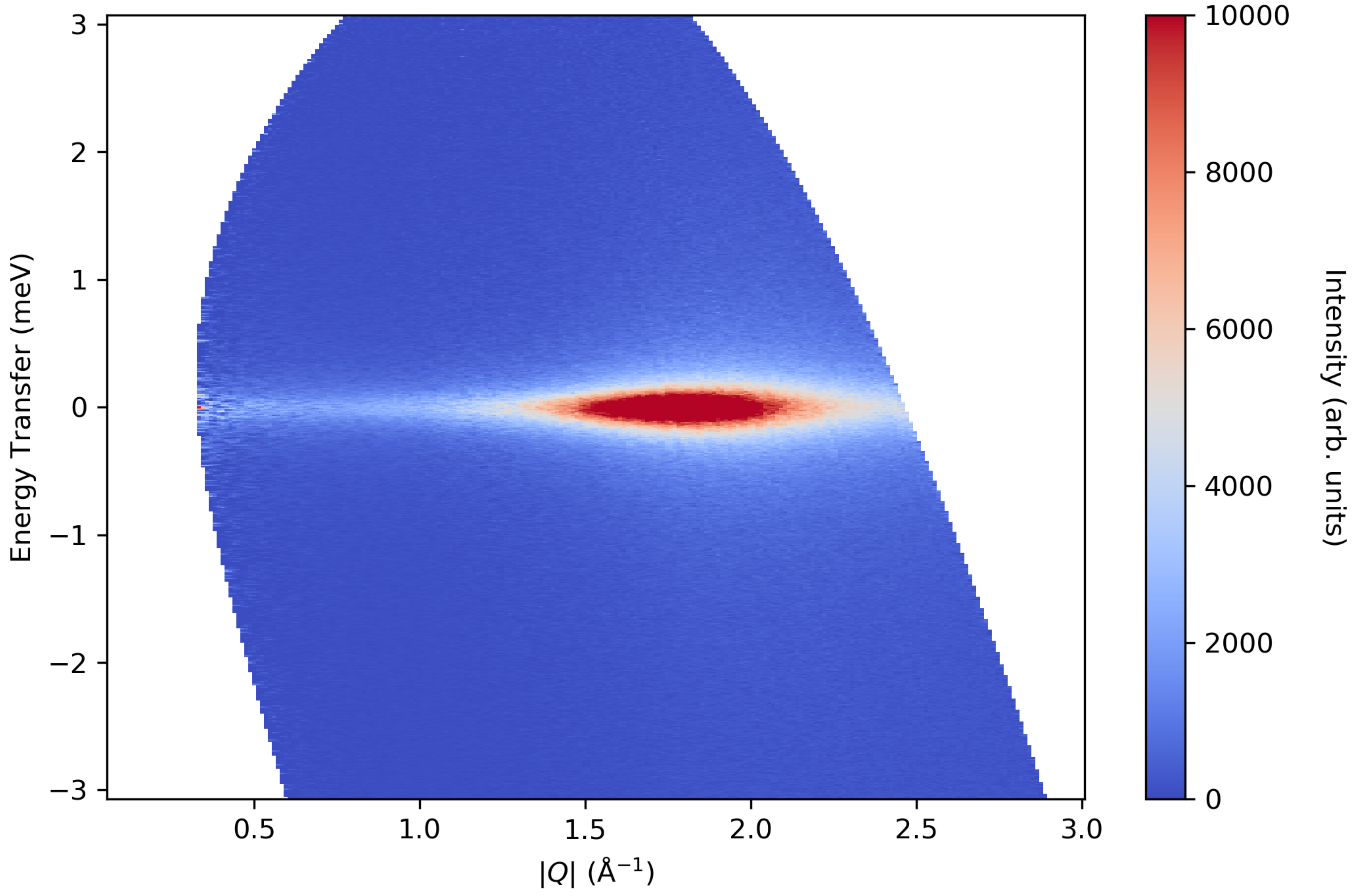
Diffusion in solvent mixtures

- Incoherent and coherent scattering from $D_2O/C_2\mathbf{H}_5OD$ mixtures: how does mixing affect hydrogen dynamics?

Incoherent



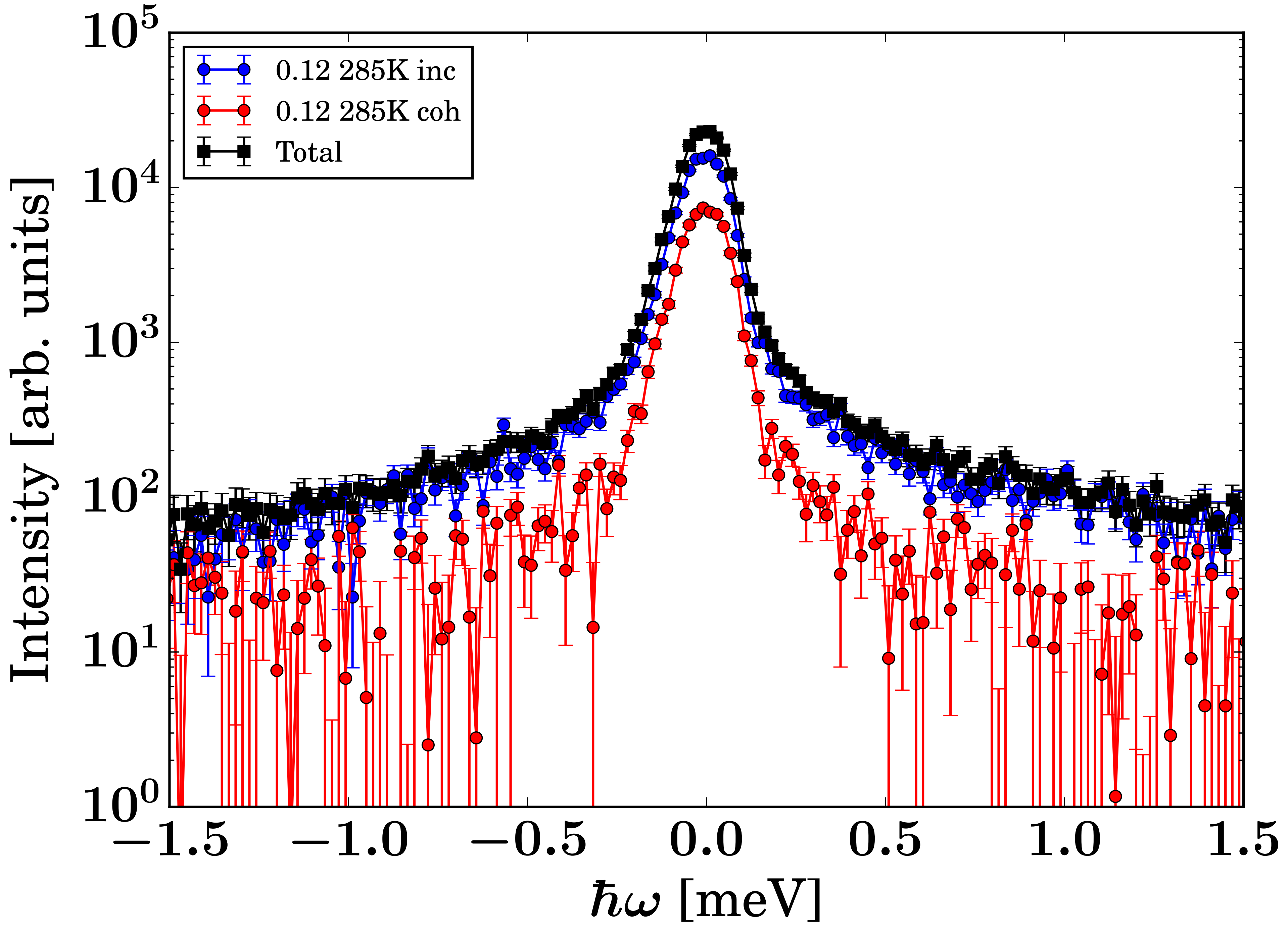
Coherent

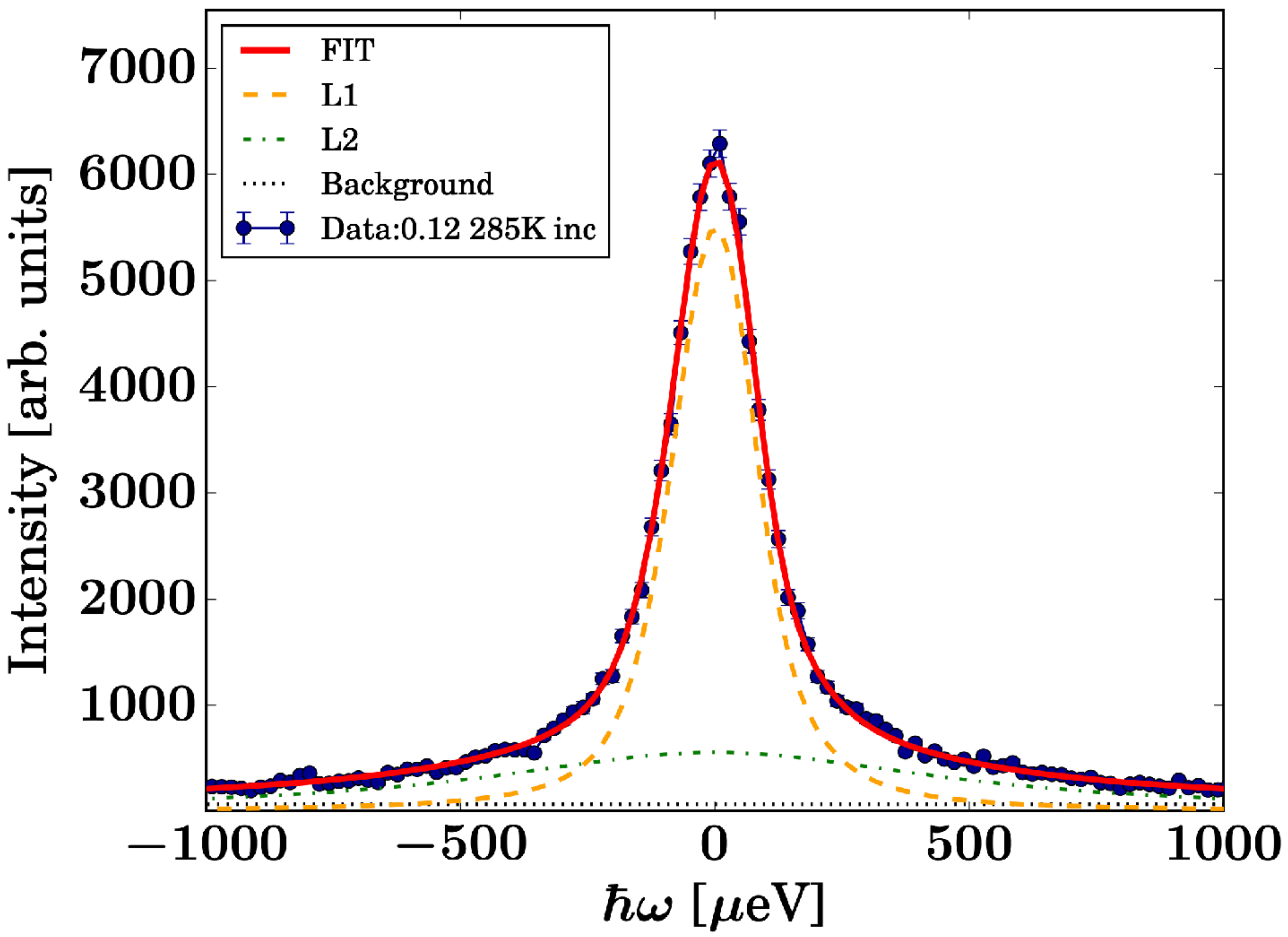


Morbidini et. al., arXiv:2310.04320v1 (2023)

Diffusion in solvent mixtures

- **Incoherent** and coherent scattering from $D_2O/C_2\mathbf{H}_5OD$ mixtures: how does mixing affect hydrogen dynamics?





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Diffusion in solvent mixtures

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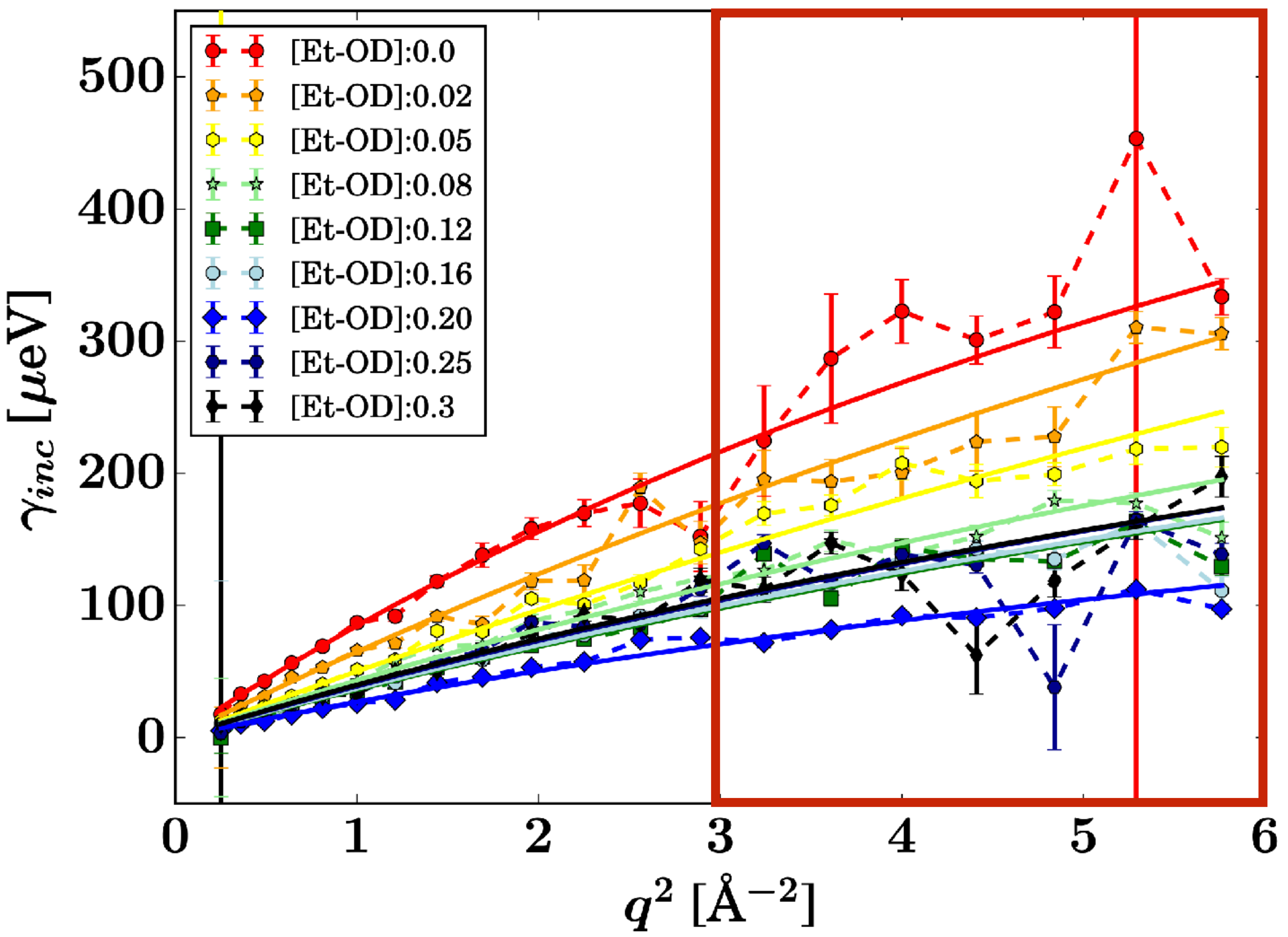
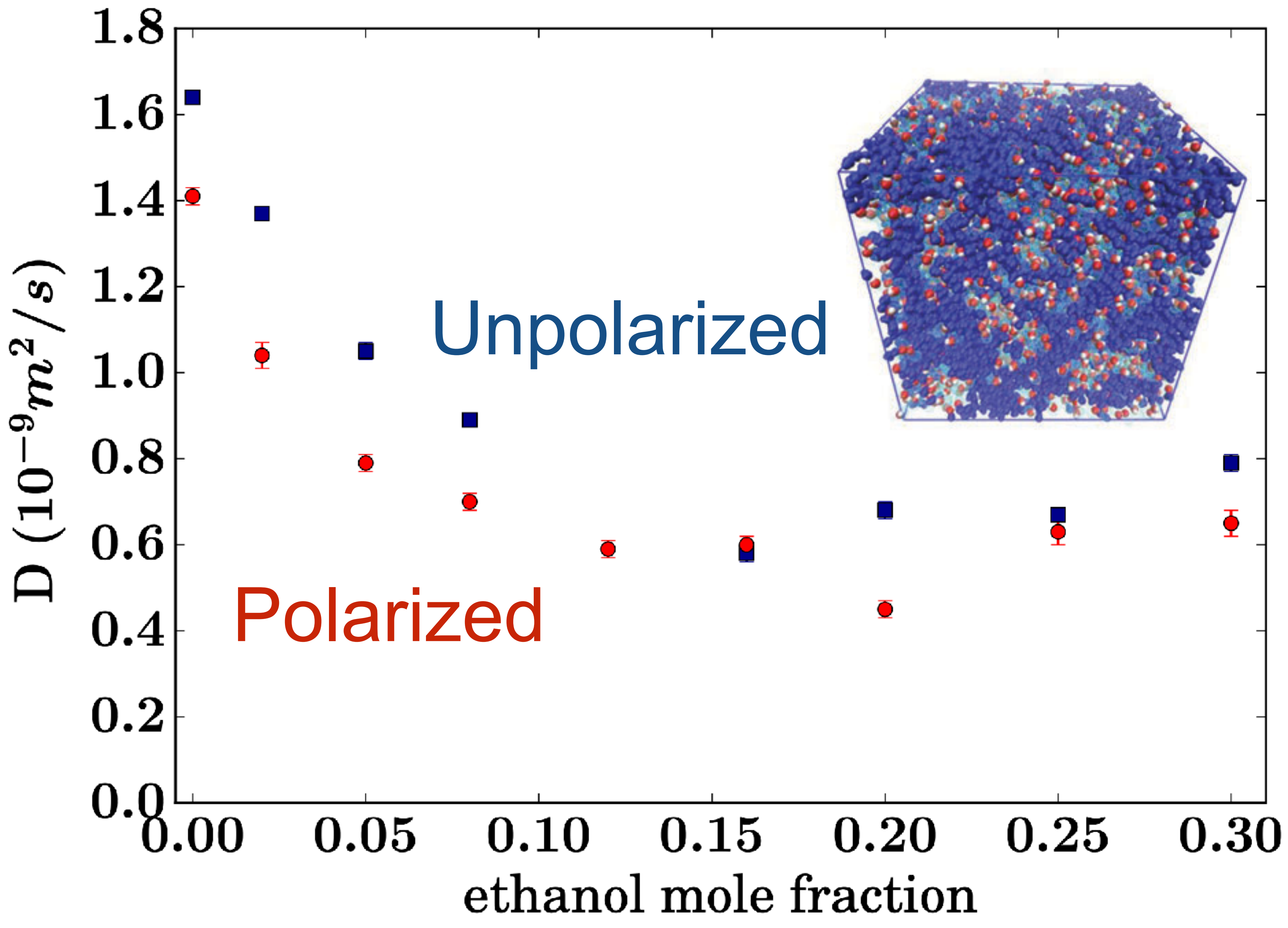


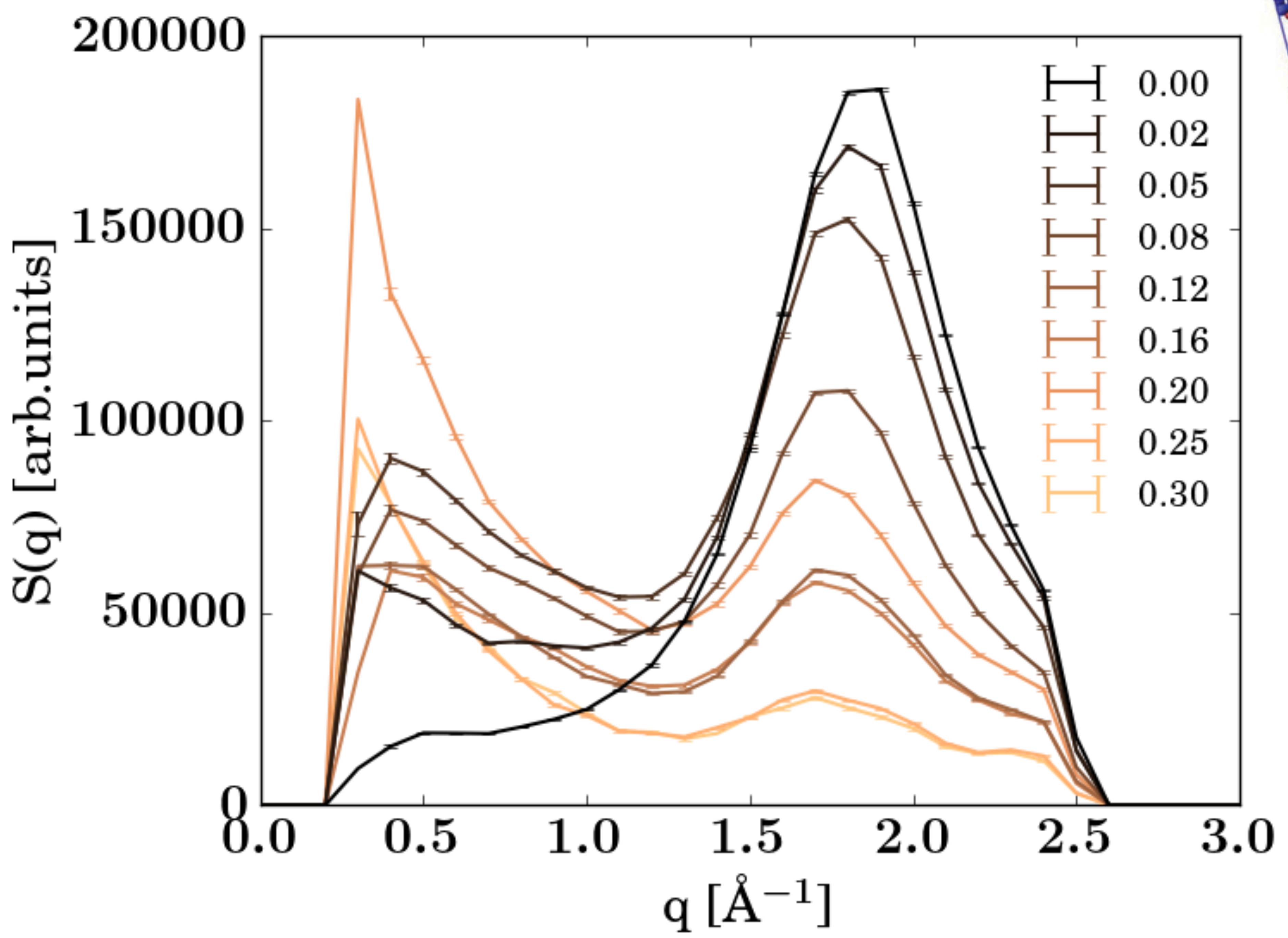


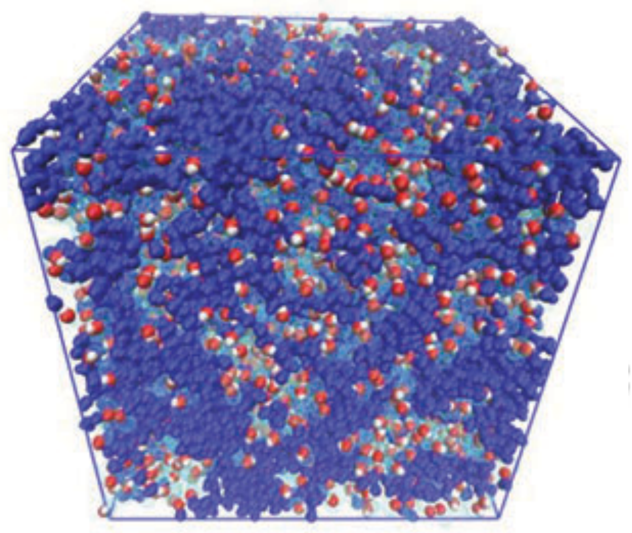
Morbidini et. al., arXiv:2310.04320v1 (2023)

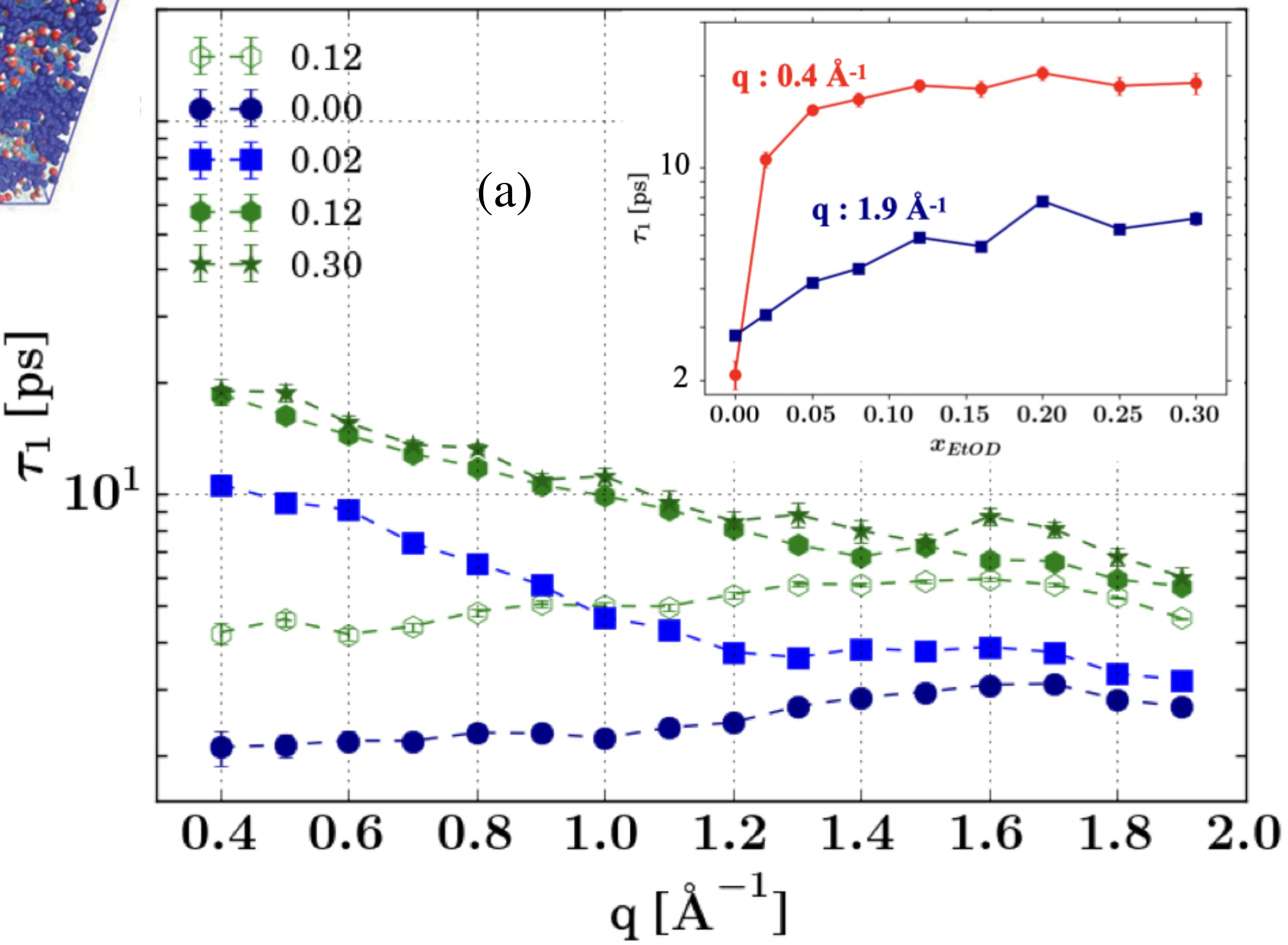
Diffusion in solvent mixtures

Science and Technology Facilities Council

- Incoherent and **coherent** scattering from $D_2O/C_2\mathbf{H_5}OD$ mixtures: what about the collective dynamics? Evidence of nanoclusters of EtOH!







Morbidini et. al., arXiv:2310.04320v1 (2023)

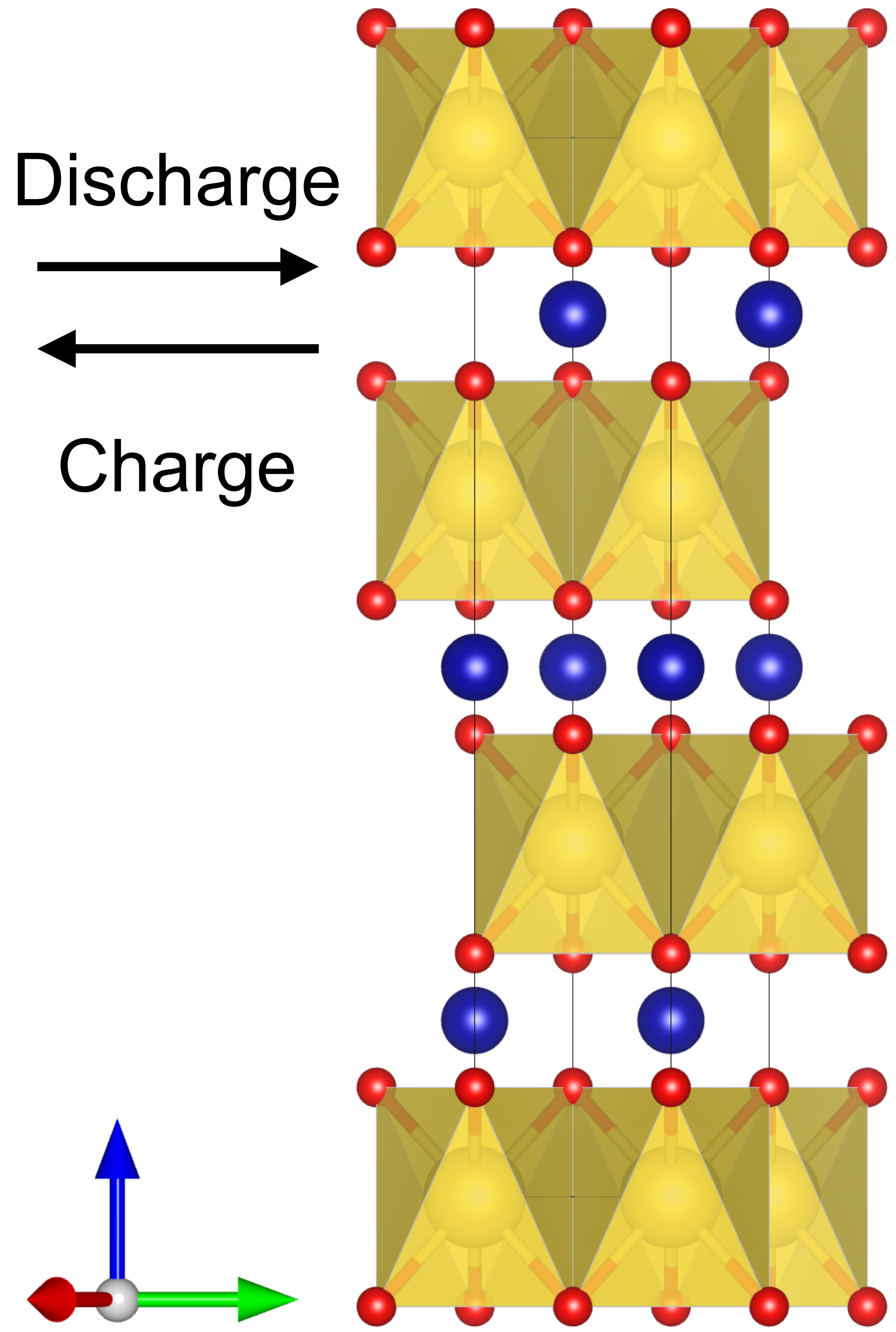
Na^+ diffusion in a candidate battery cathode material

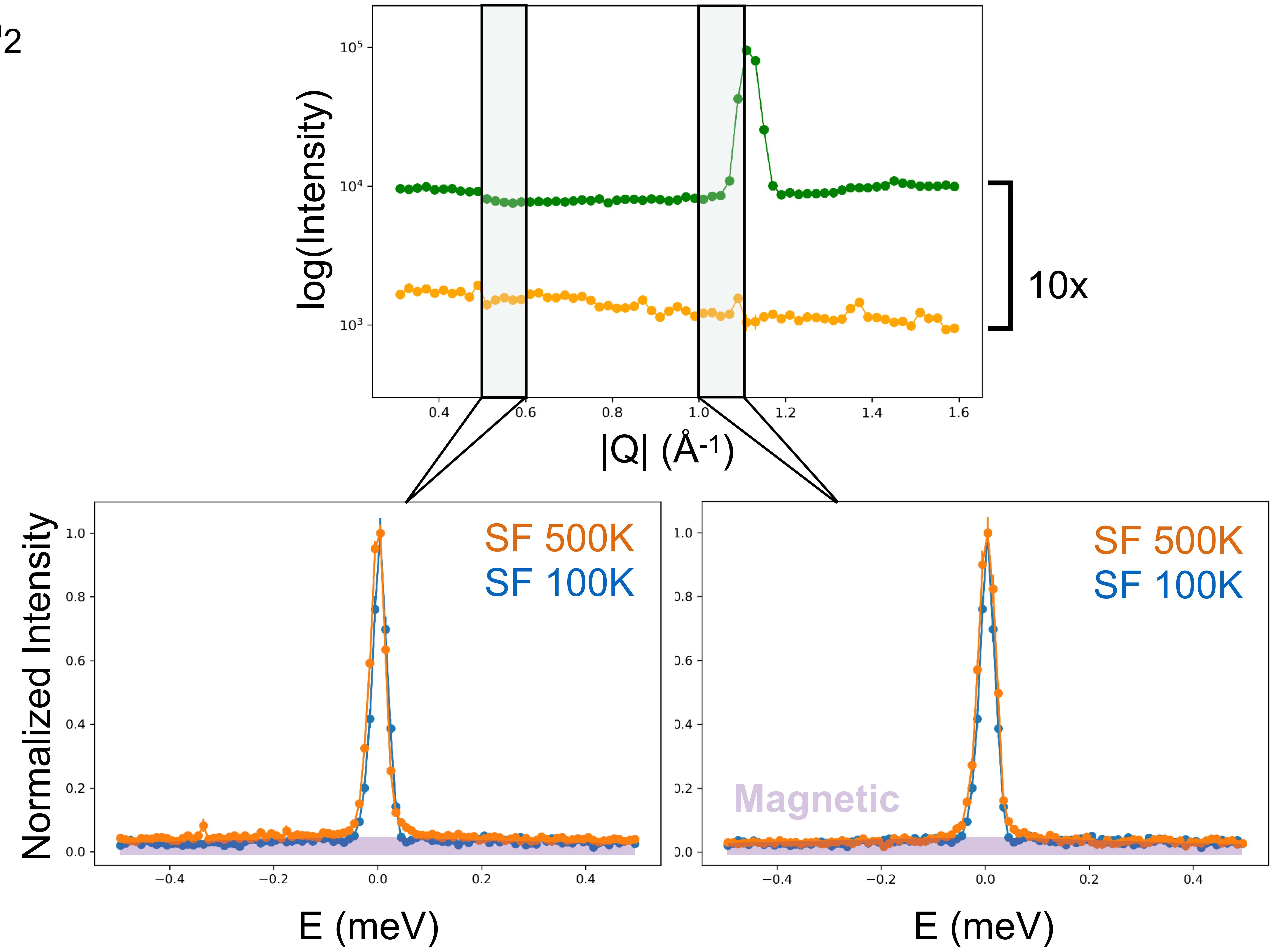
J. Goff

D. Voneshen

Na^+ diffusion in a battery cathode material

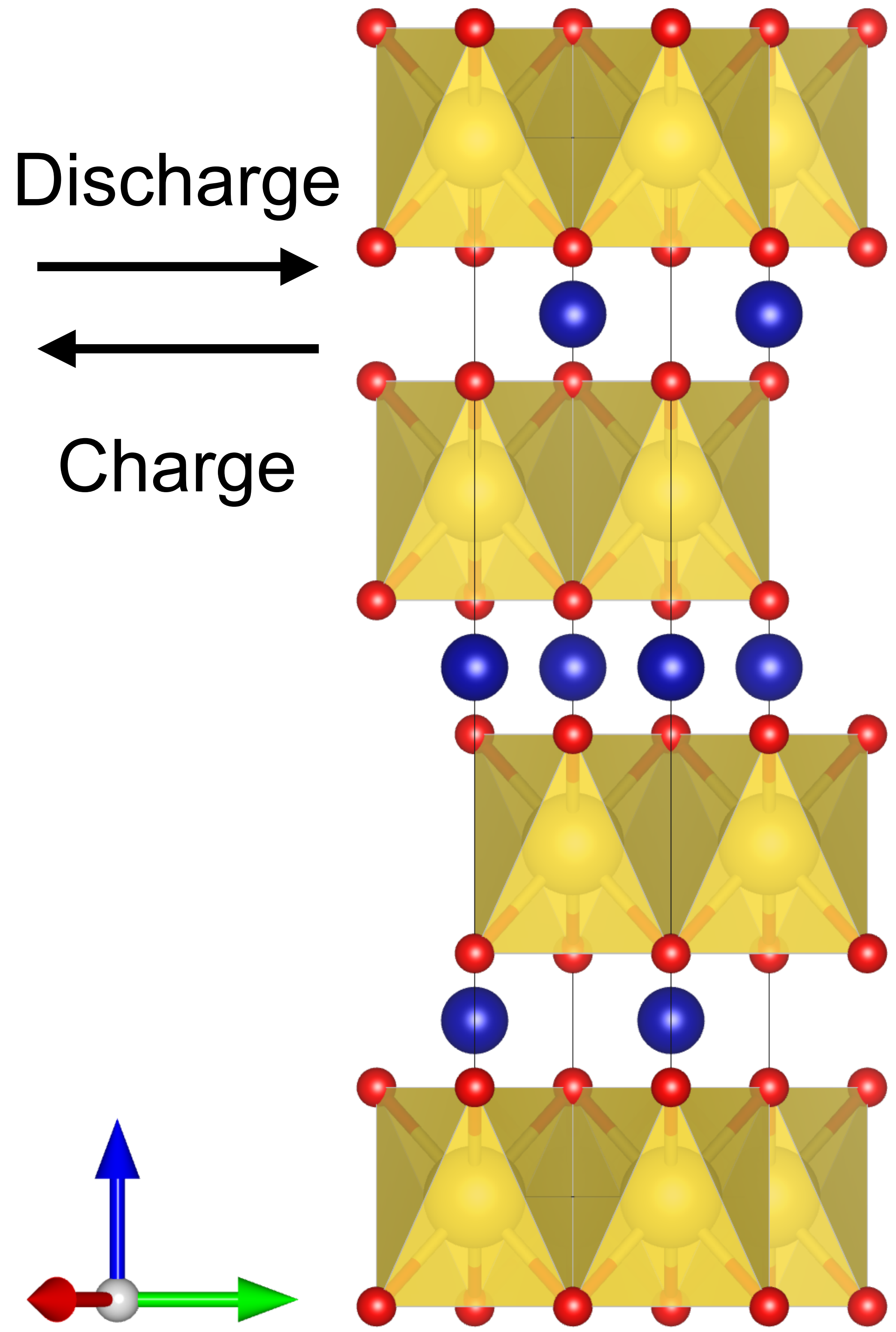
- Solid solution $NaFe_{1/2}Mn_{1/2}O_2$

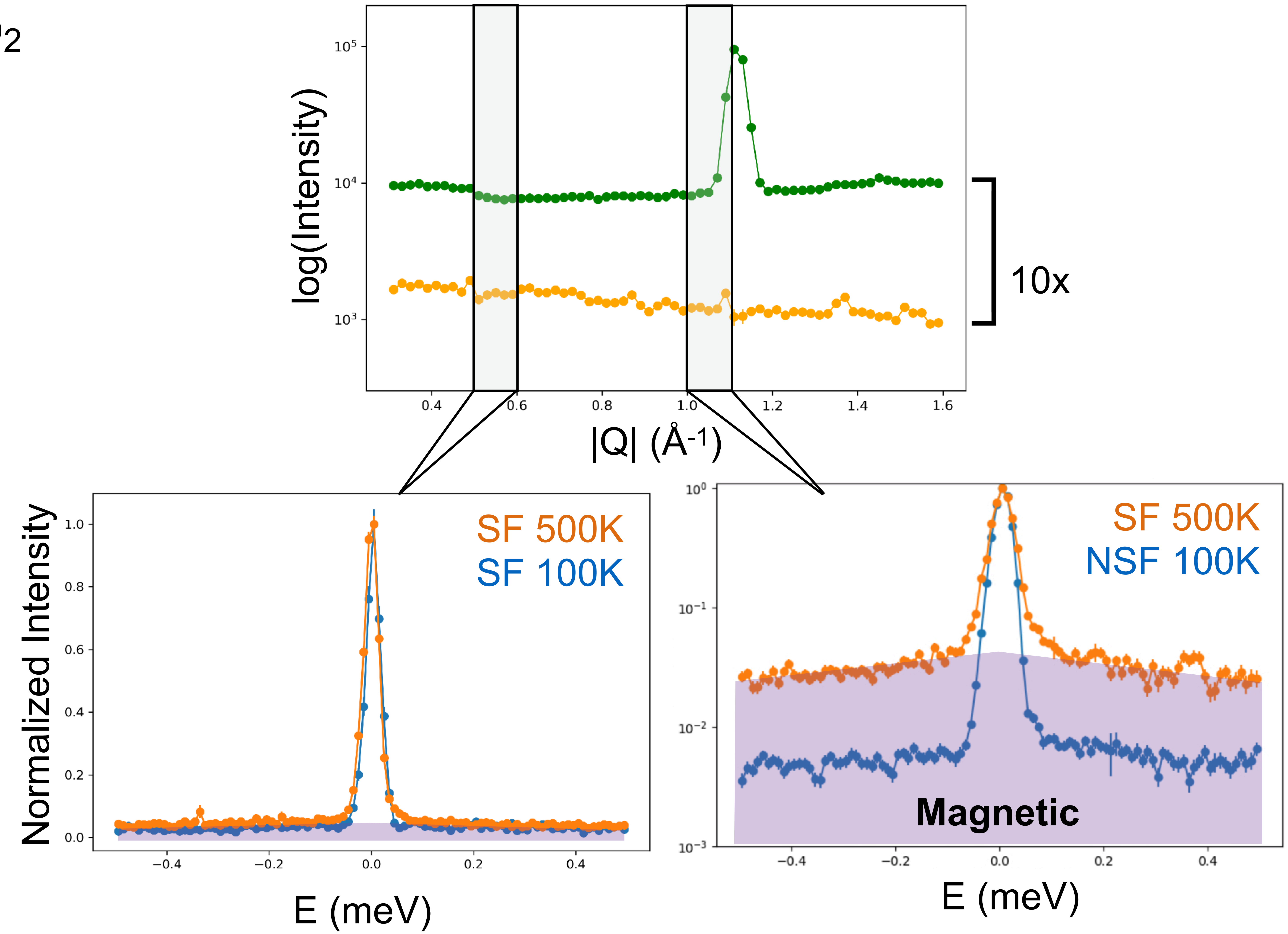




Na⁺ diffusion in a battery cathode material

- Solid solution $NaFe_{1/2}Mn_{1/2}O_2$





ROYAL HOLLOWAY UNIVERSITY OF LONDON

Science and Technology Facilities Council

Separation of magnetic component from uniaxial PA: $Ho_2Ti_2O_7$

G. Cassella

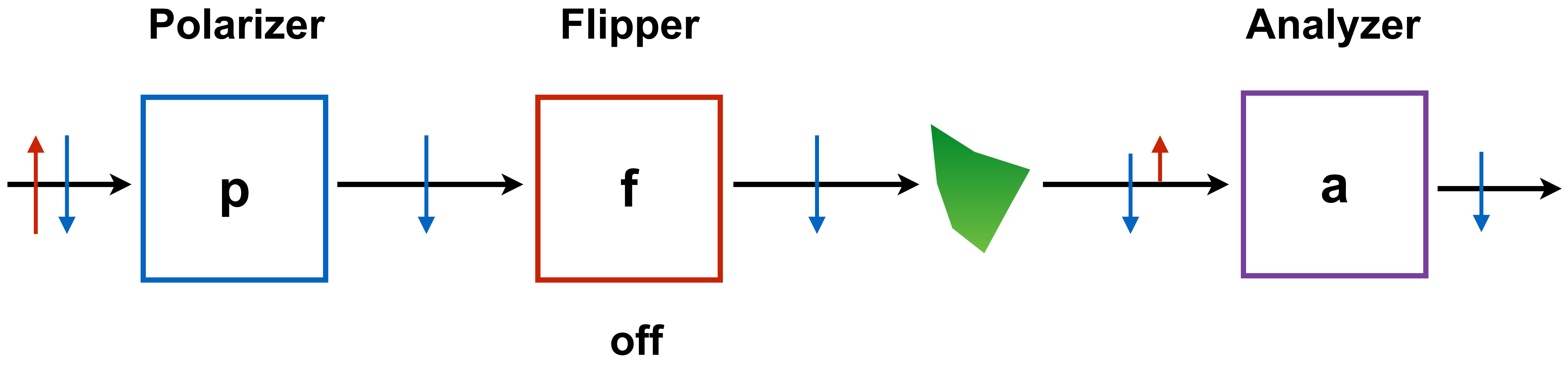
S. Arslan

J. Goff

D. Voneshen

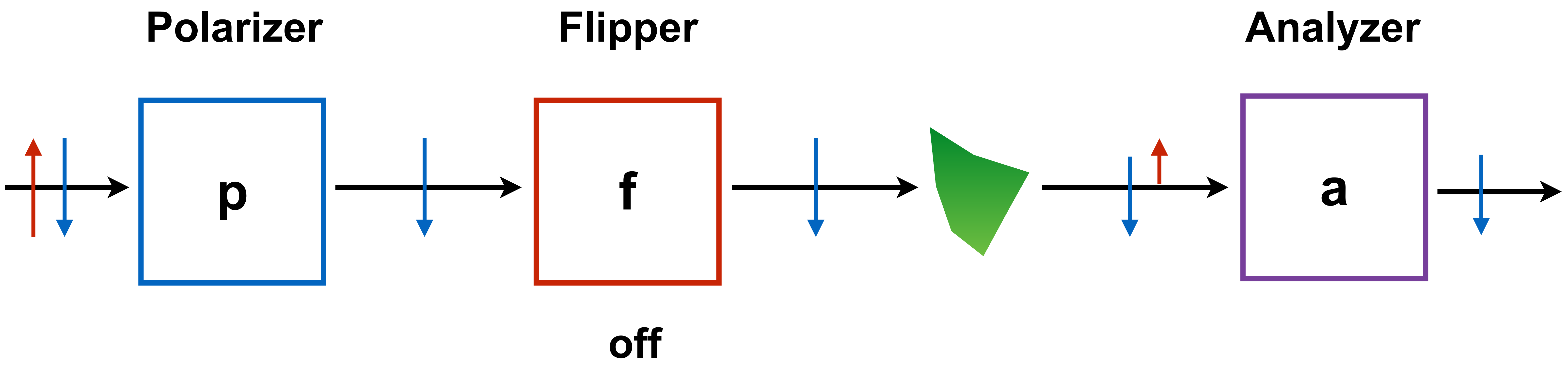
R. Perry

Longitudinal polarization analysis



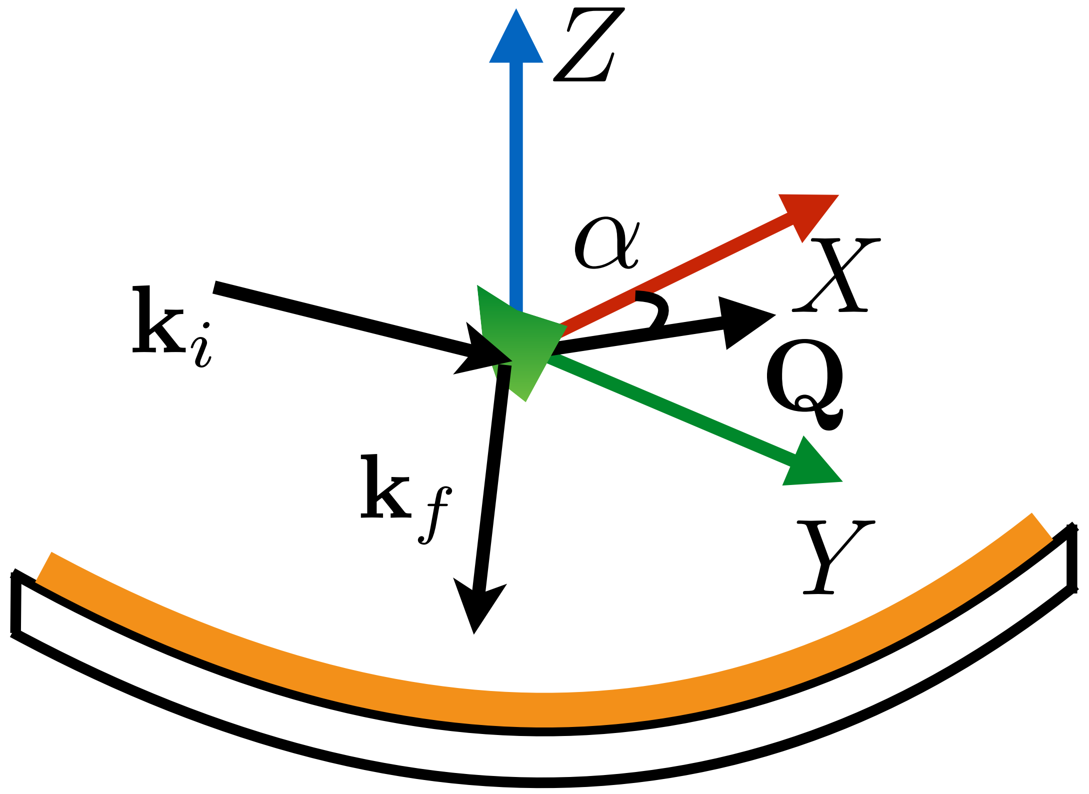
	Coherent	Spin incoherent	Paramagnetic powder	Magnetic crystal
Non spin flip	1	1/3	$\frac{1}{2}\left[1-(\hat{\mathbf{P}}\cdot\hat{\mathbf{Q}})^2\right]$	$[\hat{Q}\times M(\mathbf{Q})\times\hat{Q}]_{\|\|\mathbf{P}}$
Spin flip	0	2/3	$\frac{1}{2}\left[1+(\hat{\mathbf{P}}\cdot\hat{\mathbf{Q}})^2\right]$	$[\hat{Q}\times M(\mathbf{Q})\times\hat{Q}]_{\perp\mathbf{P}}$

Longitudinal polarization analysis



	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\text{coh}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\text{inc}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\text{mag}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\text{mag}}$
$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{--}$	1	1/3	$\frac{1}{2}\left[1-(\hat{\mathbf{P}}\cdot\hat{\mathbf{Q}})^2\right]$	$[\hat{Q}\times M(\mathbf{Q})\times\hat{Q}]_{\vert\vert\mathbf{P}}$
$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{+-}$	0	2/3	$\frac{1}{2}\left[1+(\hat{\mathbf{P}}\cdot\hat{\mathbf{Q}})^2\right]$	$[\hat{Q}\times M(\mathbf{Q})\times\hat{Q}]_{\perp\mathbf{P}}$

XYZ method: paramagnetic powder

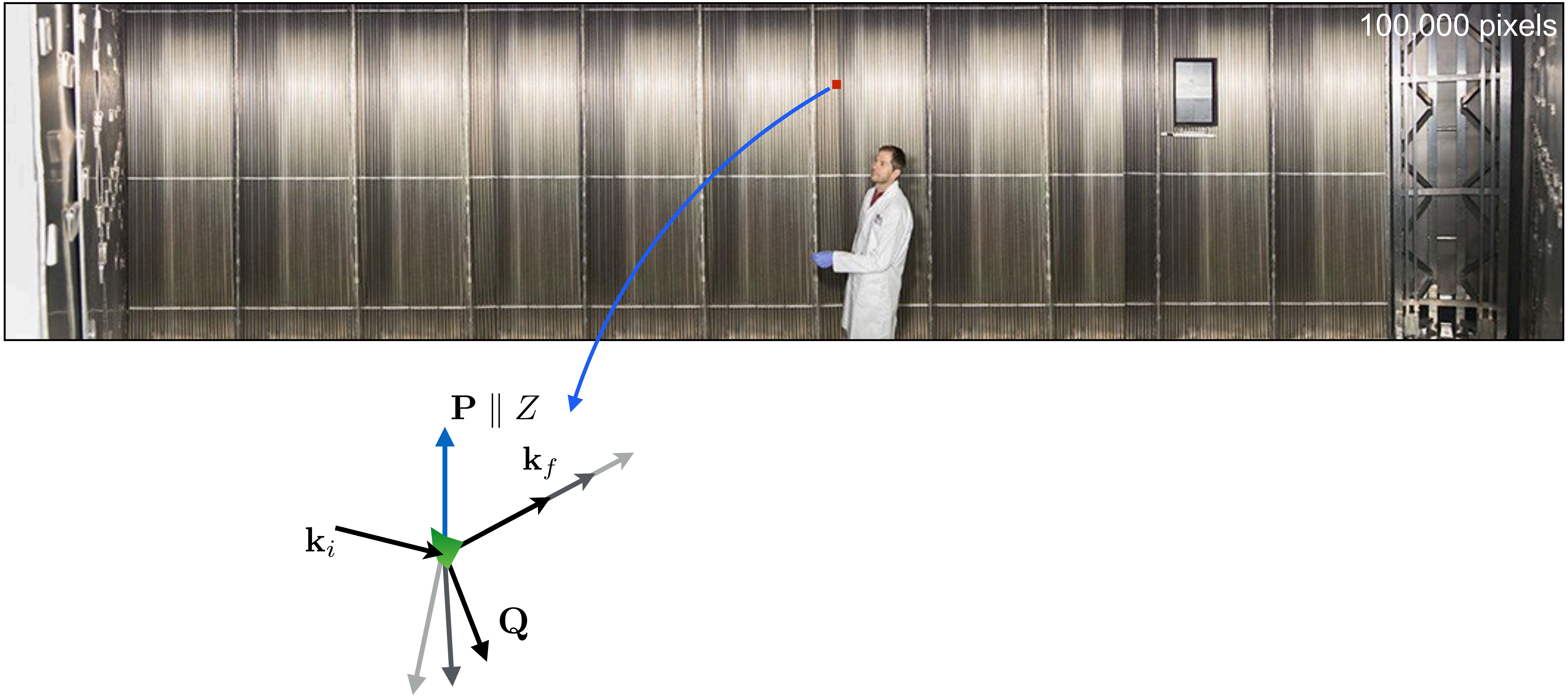


$$\frac{1}{2}\left[1 - (\hat{\mathbf{P}} \cdot \hat{\mathbf{Q}})^2\right]$$

	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\mathrm{coh}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\mathrm{inc}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\mathrm{mag}}^{X}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\mathrm{mag}}^{Y}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\mathrm{mag}}^{Z}$
$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{--}$	1	1/3	$\frac{1}{2}\sin^2\alpha$	$\frac{1}{2}\cos^2\alpha$	$\frac{1}{2}$
$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{+-}$	0	2/3	$\frac{1}{2}(\cos^2\alpha + 1)$	$\frac{1}{2}(\sin^2\alpha + 1)$	$\frac{1}{2}$

Schärpf and Capellmann, PSSA **135**, 359 (1993)

Uniaxial PA with a PSD



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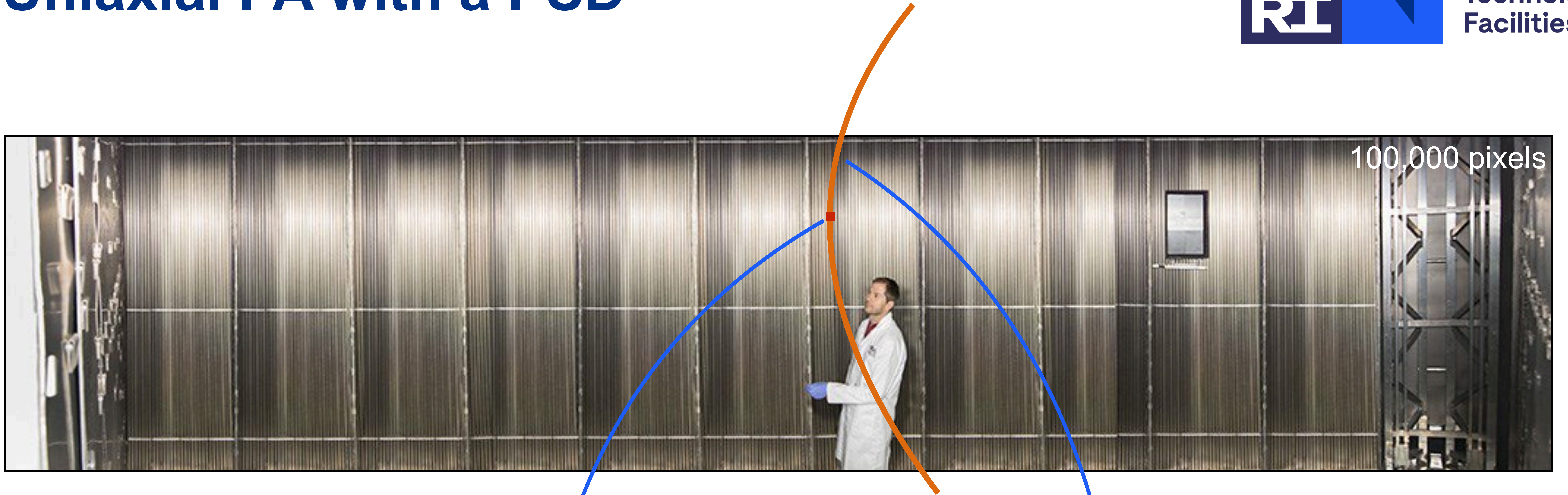
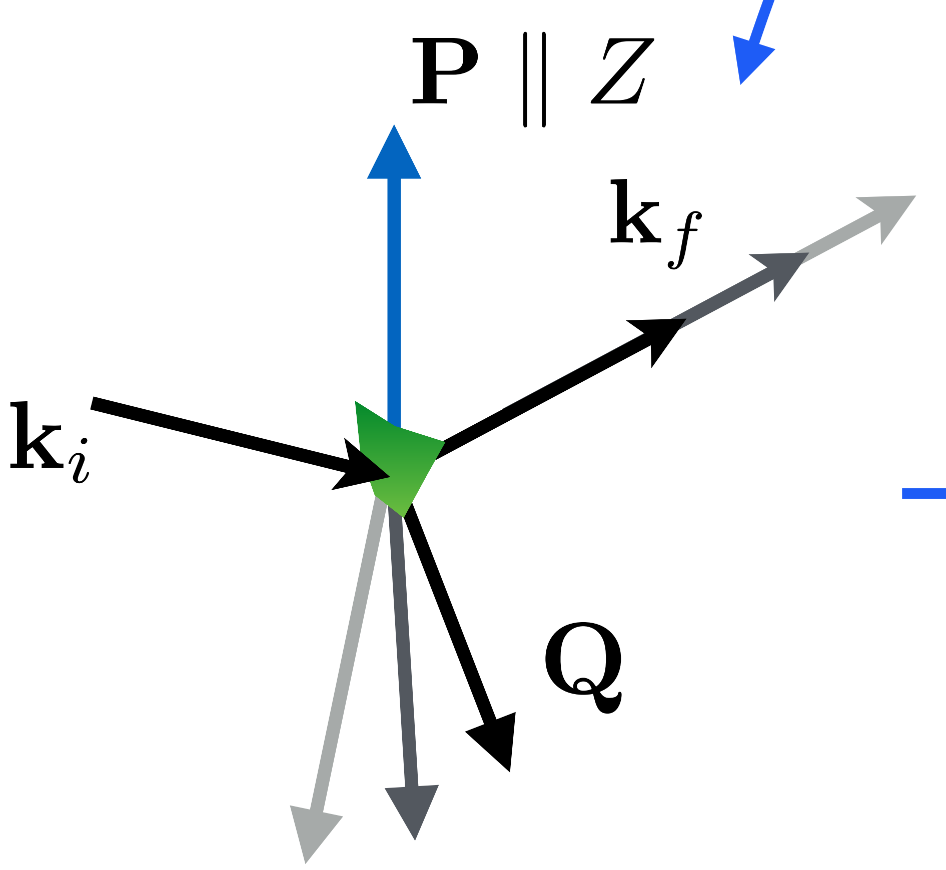
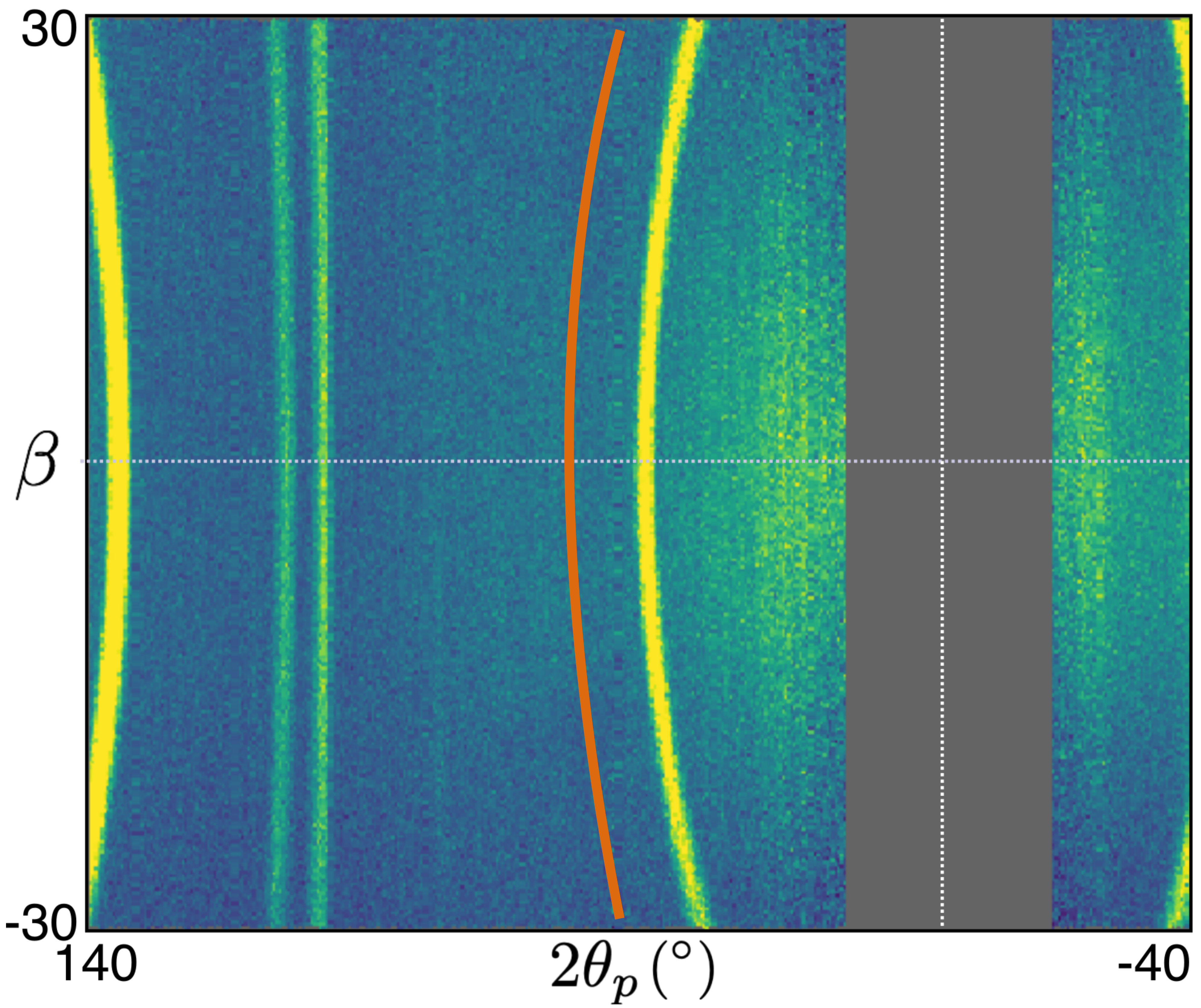


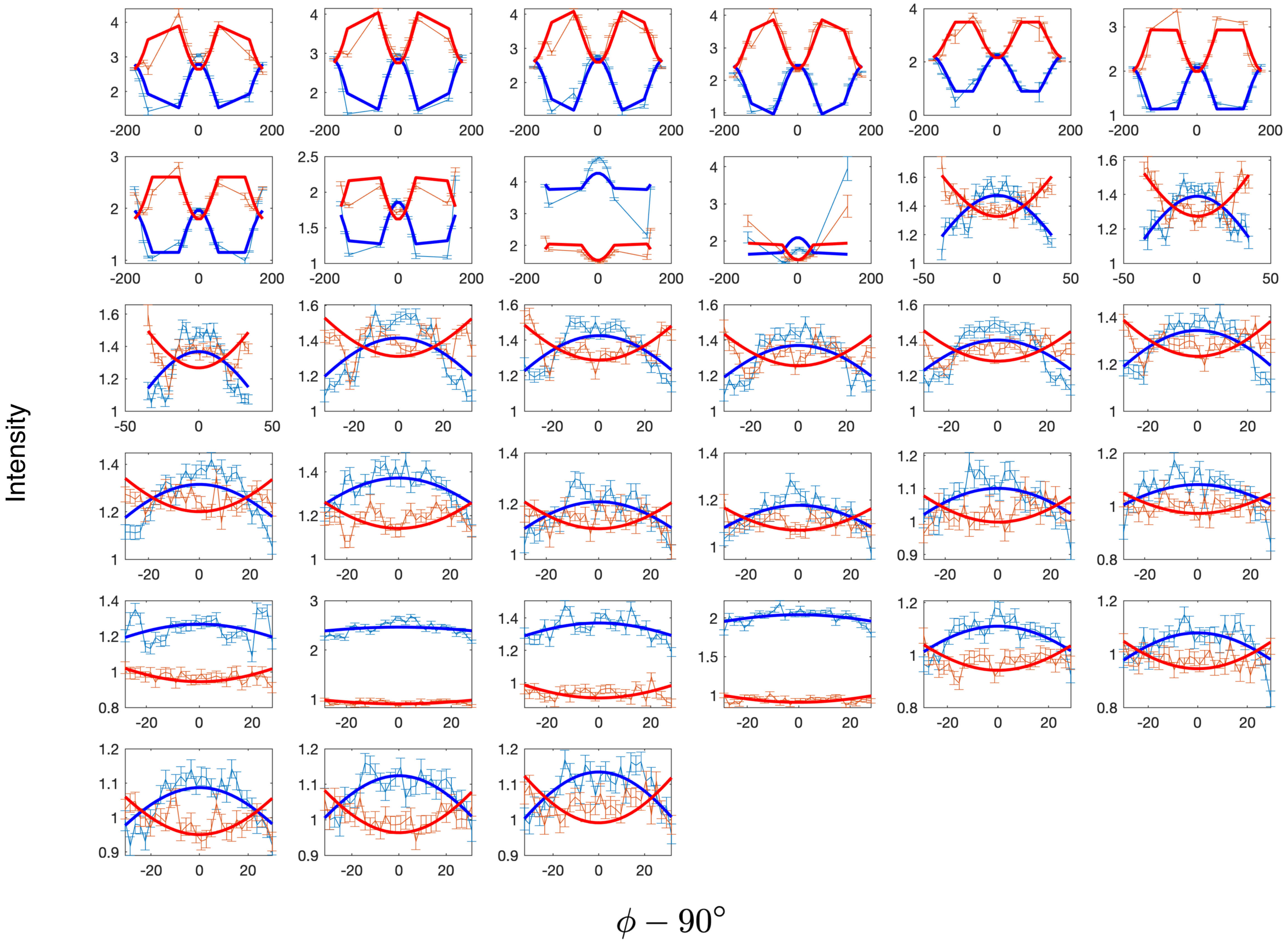


$$> 10,000 \ (|Q|, E, (\mathbf{P}\cdot\mathbf{Q})^2)$$

z+: experimental separation

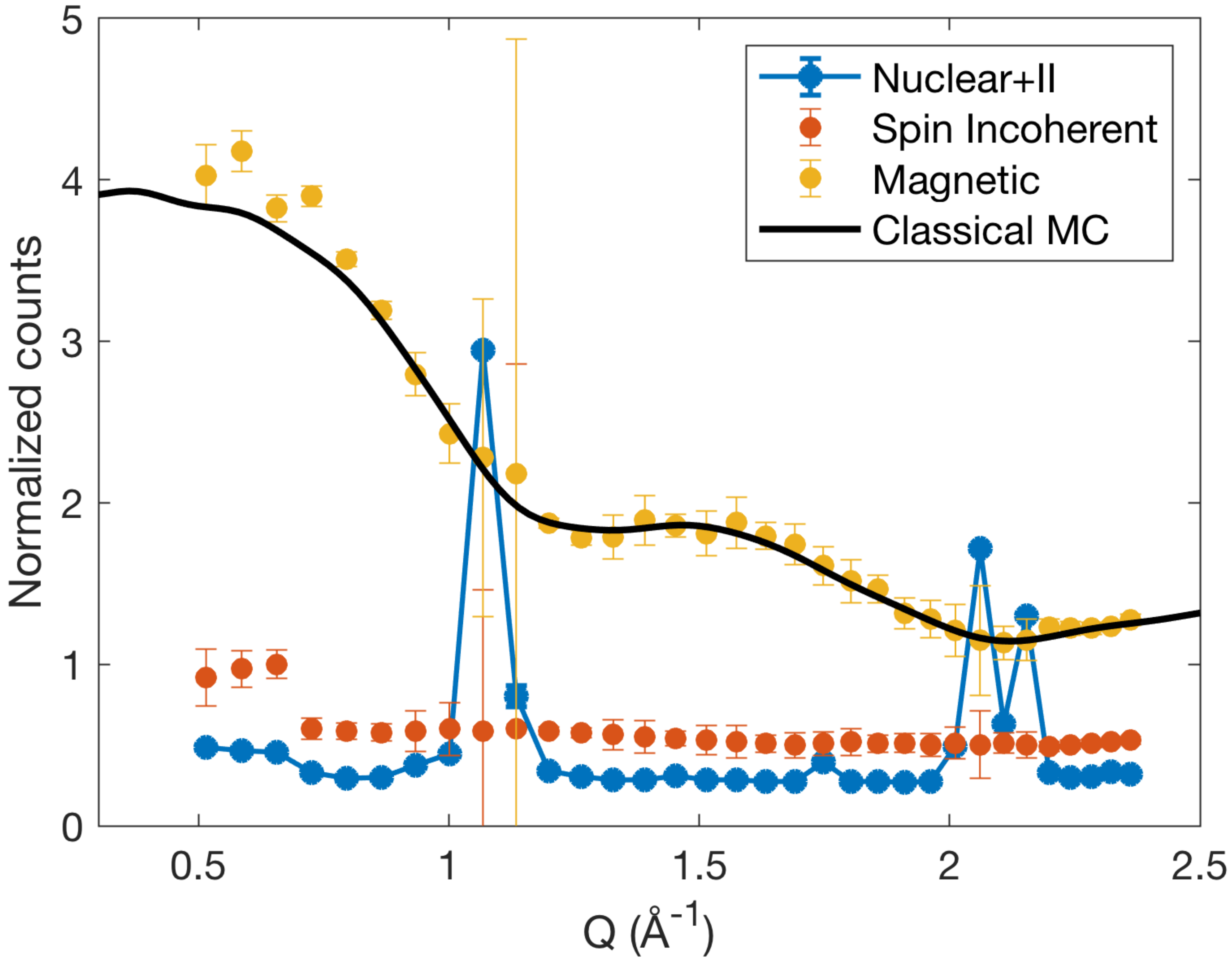
- *e.g.* $Ho_2Ti_2O_7$ (“spin ice”) - elastic scattering from LET





G. J. Nilsen et al., Rev. Sci. Instrum. **93** (6), 063902 (2022)

z+: experimental separation



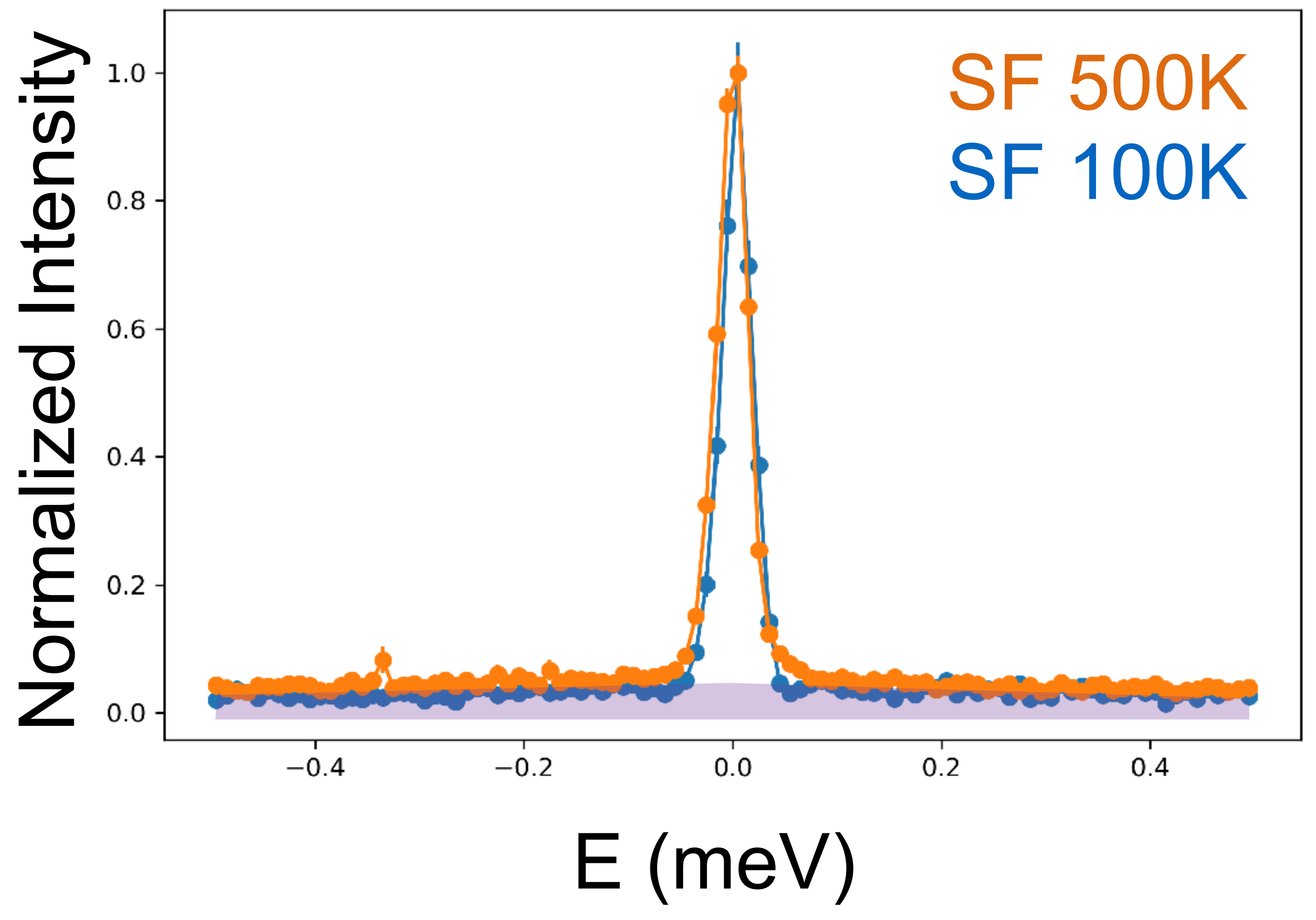
G. J. Nilsen et al., Rev. Sci. Instrum. **93** (6), 063902 (2022)

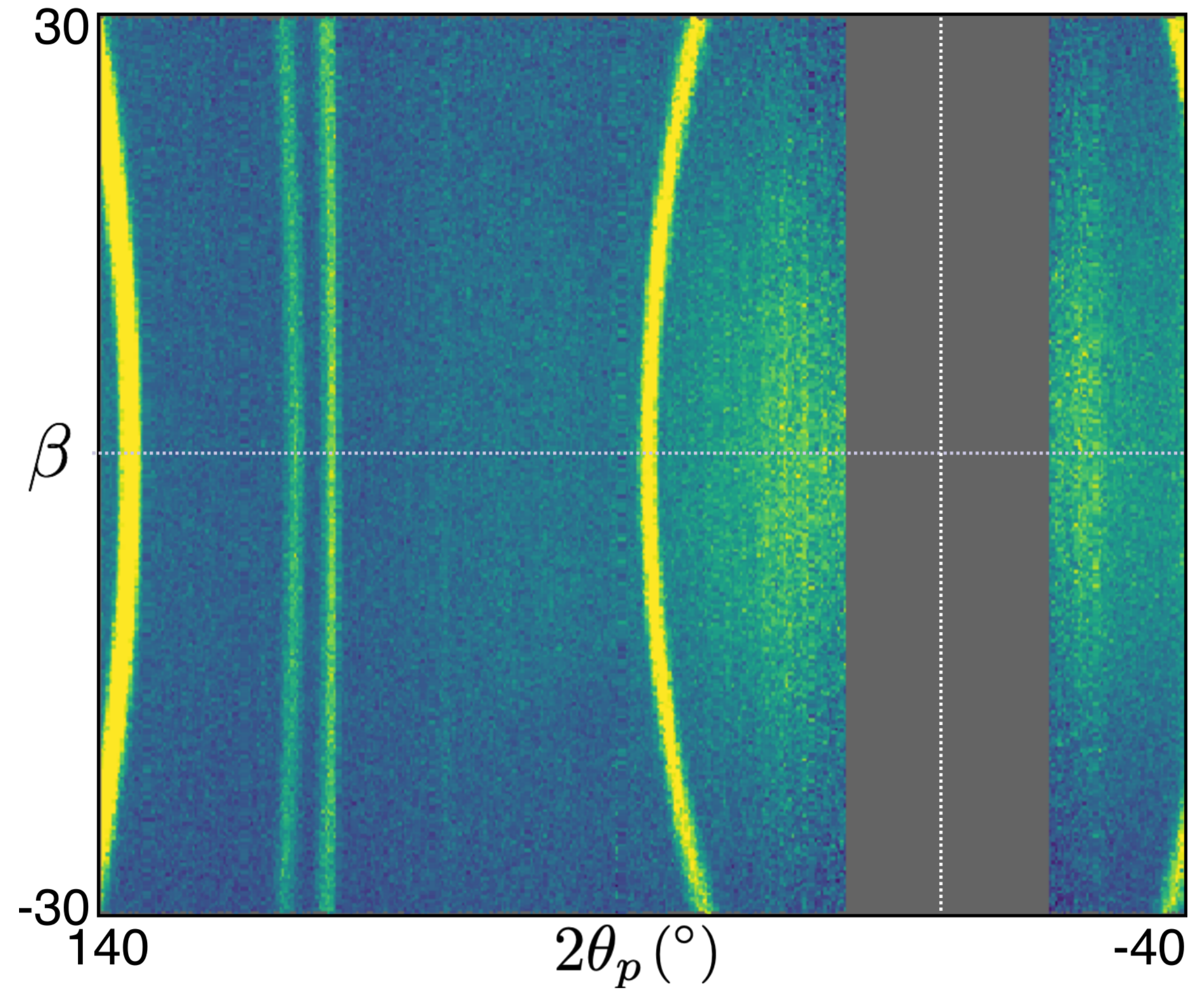
Conclusions and future prospects

- Polarized TOF has shown its potential for QENS (and INS) on a range of systems
- Crucial when looking for weak scattering, complex systems, or coherent QENS
- Technology mature to increase complexity
- z+ shows promise, but limited by statistics and works best at small *Q*

  → **XYZ polarized diffraction**
- Also, need high count rate at high resolution:

  → **Indirect/backscattering**





Endeavour

Future: Wide-angle XYZ PA on WISH

WISH diffractometer

- WISH: large *d*-spacing neutron diffractometer
  - Solid CH_4 moderator
  - Leading instrument:
    - *m* = 3 double elliptical guide
    - 340° in-plane detector coverage
    - Optimised for powders, but can measure single crystals
    - >50% magnetic samples

Photo: Max Alexander

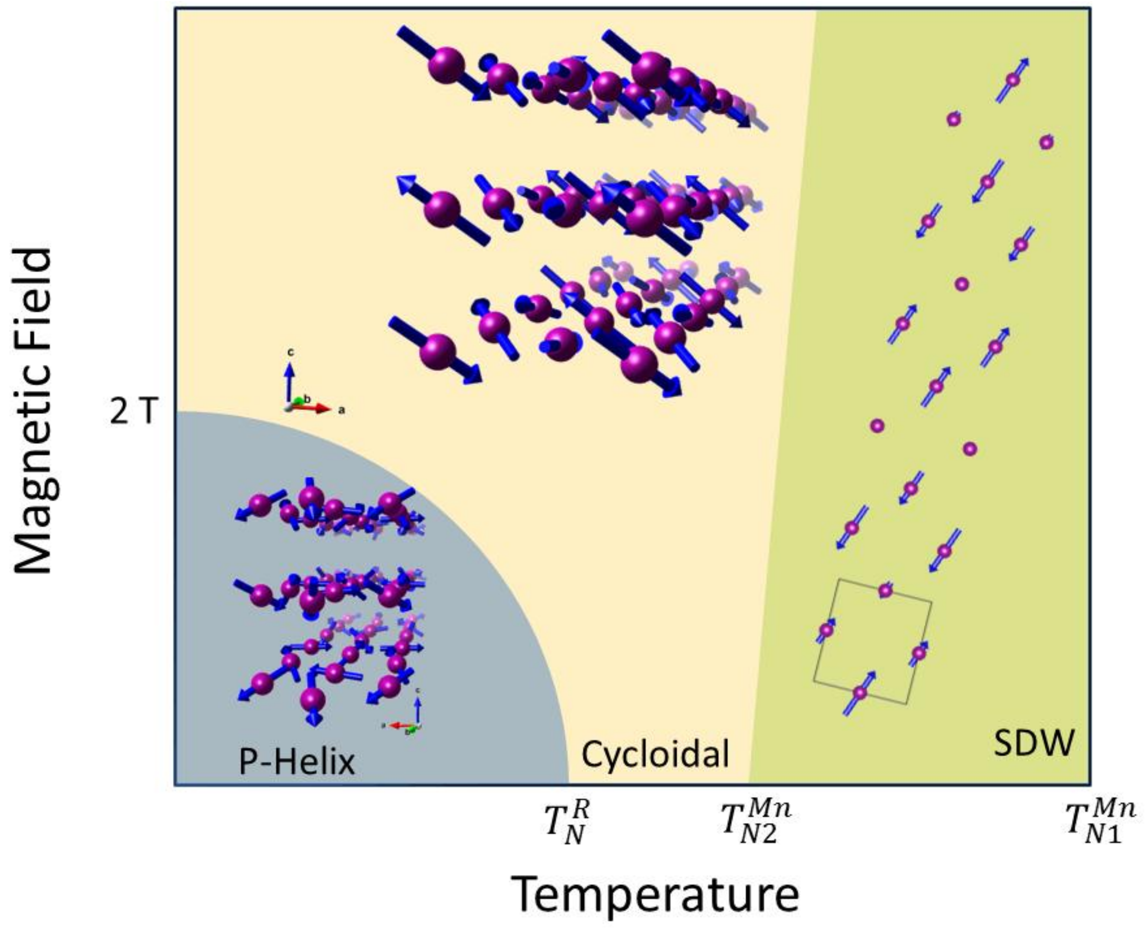
Science case

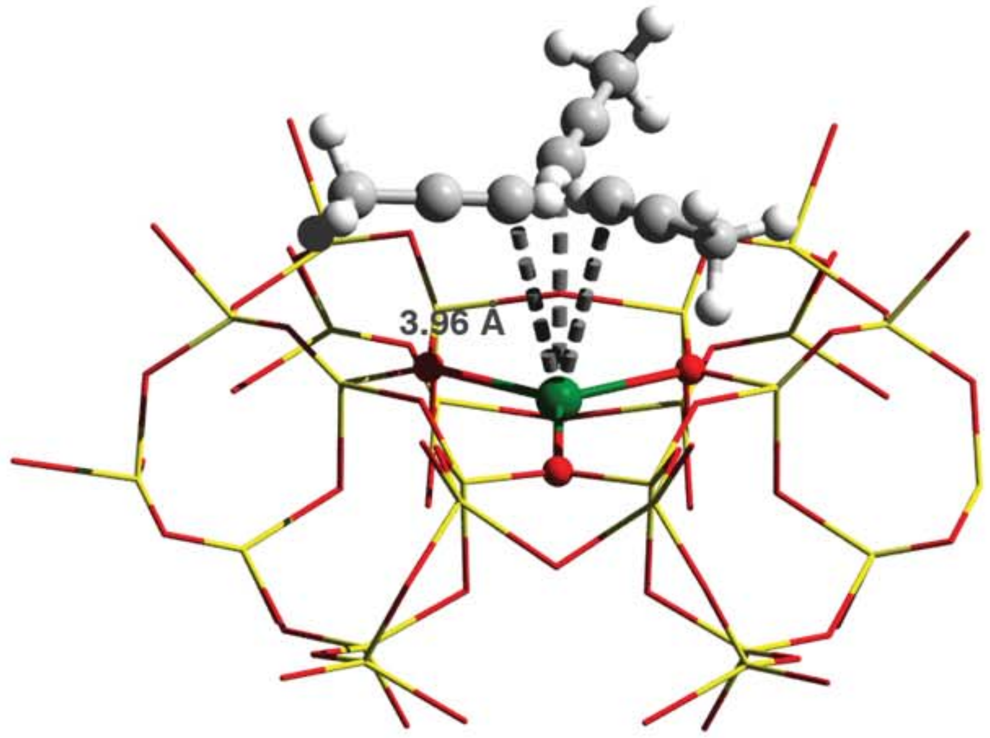
Powder

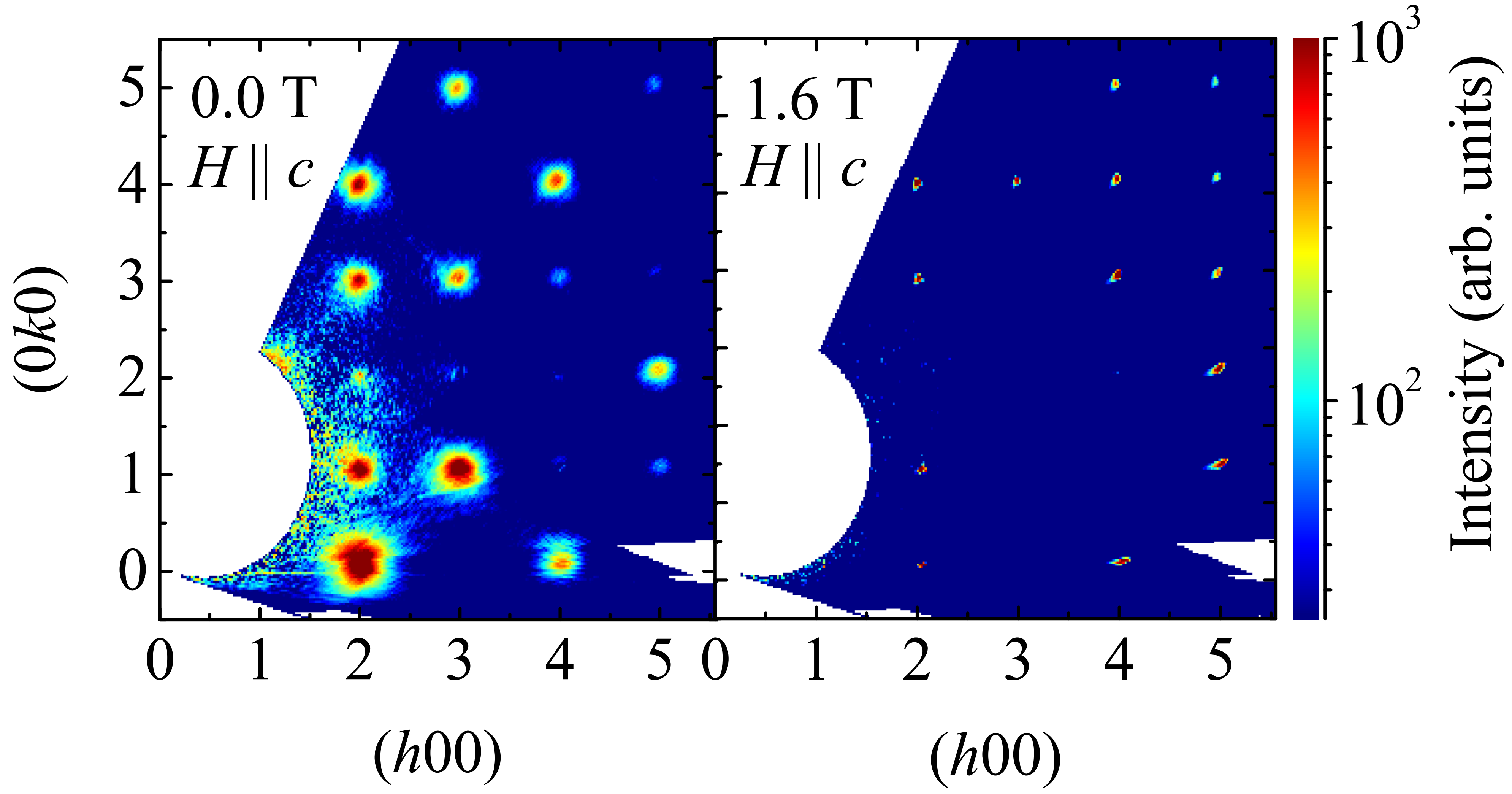
Single crystal

Magnetic

Non-magnetic



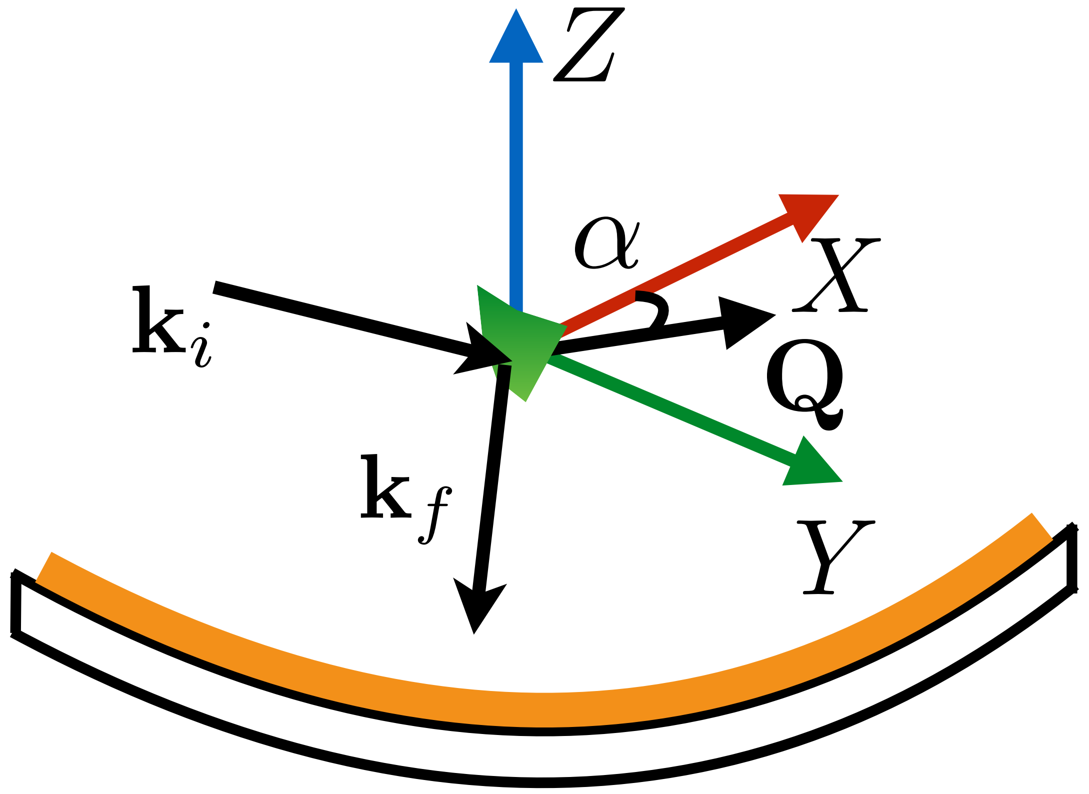




PRM **3**, 044401 (2019) Chai et al.Science **368**, 1002 (2020) O. Young *et al.*, PRB **88**, 024411 (2013)

Complex magnetic order, weak moments, diffuse scattering, large unit cells

XYZ method: paramagnetic powder



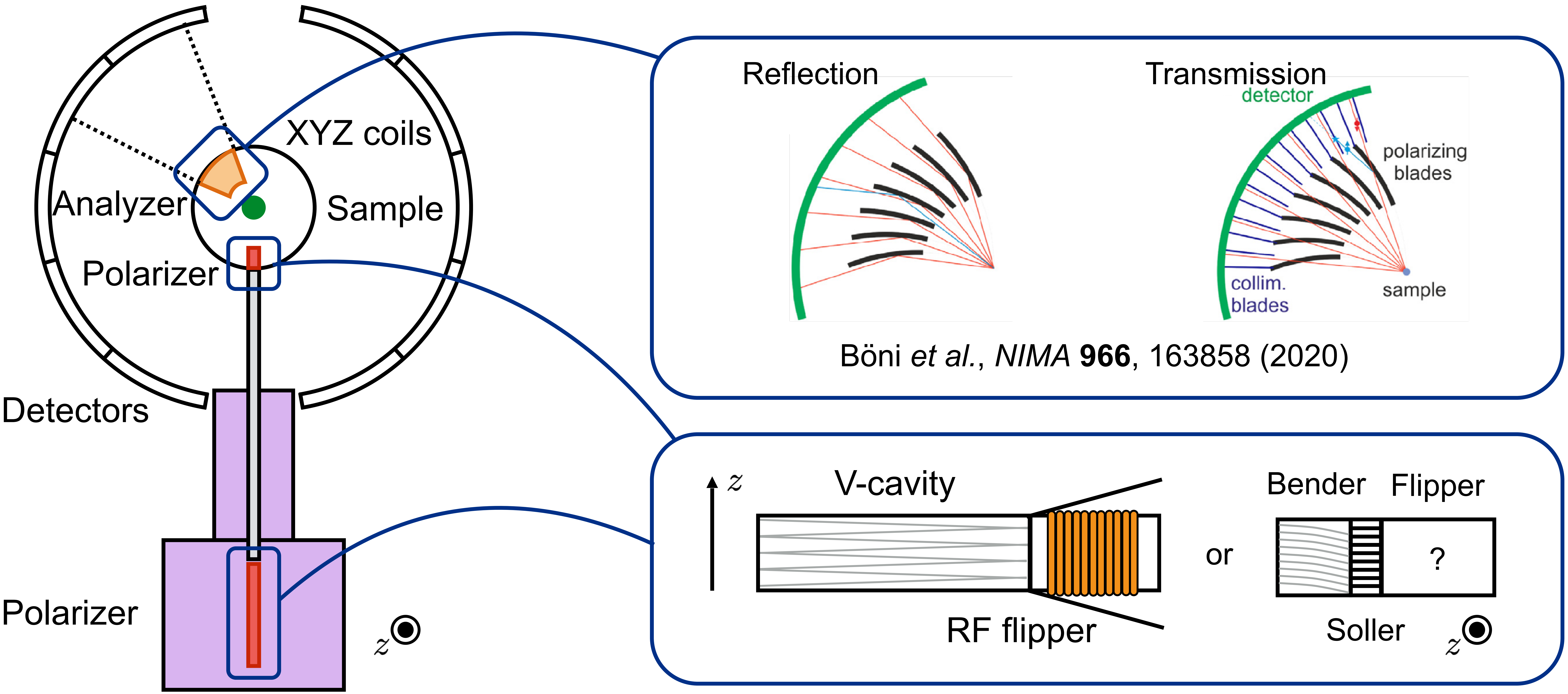
$$\frac{1}{2}\left[1-(\hat{\mathbf{P}}\cdot\hat{\mathbf{Q}})^2\right]$$

	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\text{coh}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{\text{inc}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)^X_{\text{mag}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)^Y_{\text{mag}}$	$\left(\frac{d^2\sigma}{d\Omega dE}\right)^Z_{\text{mag}}$
$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{--}$	1	1/3	$\frac{1}{2}\sin^2\alpha$	$\frac{1}{2}\cos^2\alpha$	$\frac{1}{2}$
$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{+-}$	0	2/3	$\frac{1}{2}(\cos^2\alpha+1)$	$\frac{1}{2}(\sin^2\alpha+1)$	$\frac{1}{2}$

Schärpf and Capellmann, PSSA **135**, 359 (1993)

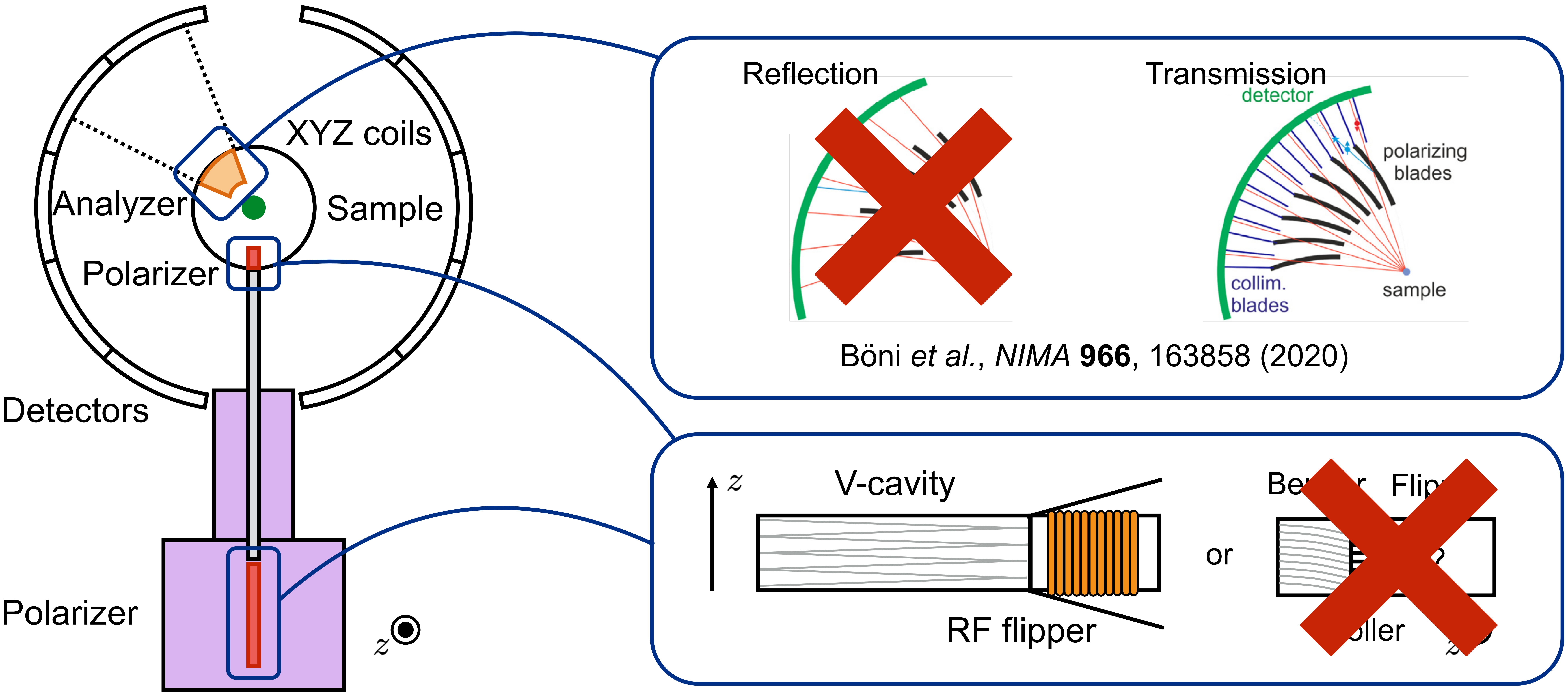
WISH: Instrument layout

Science and Technology Facilities Council



WISH: Instrument layout

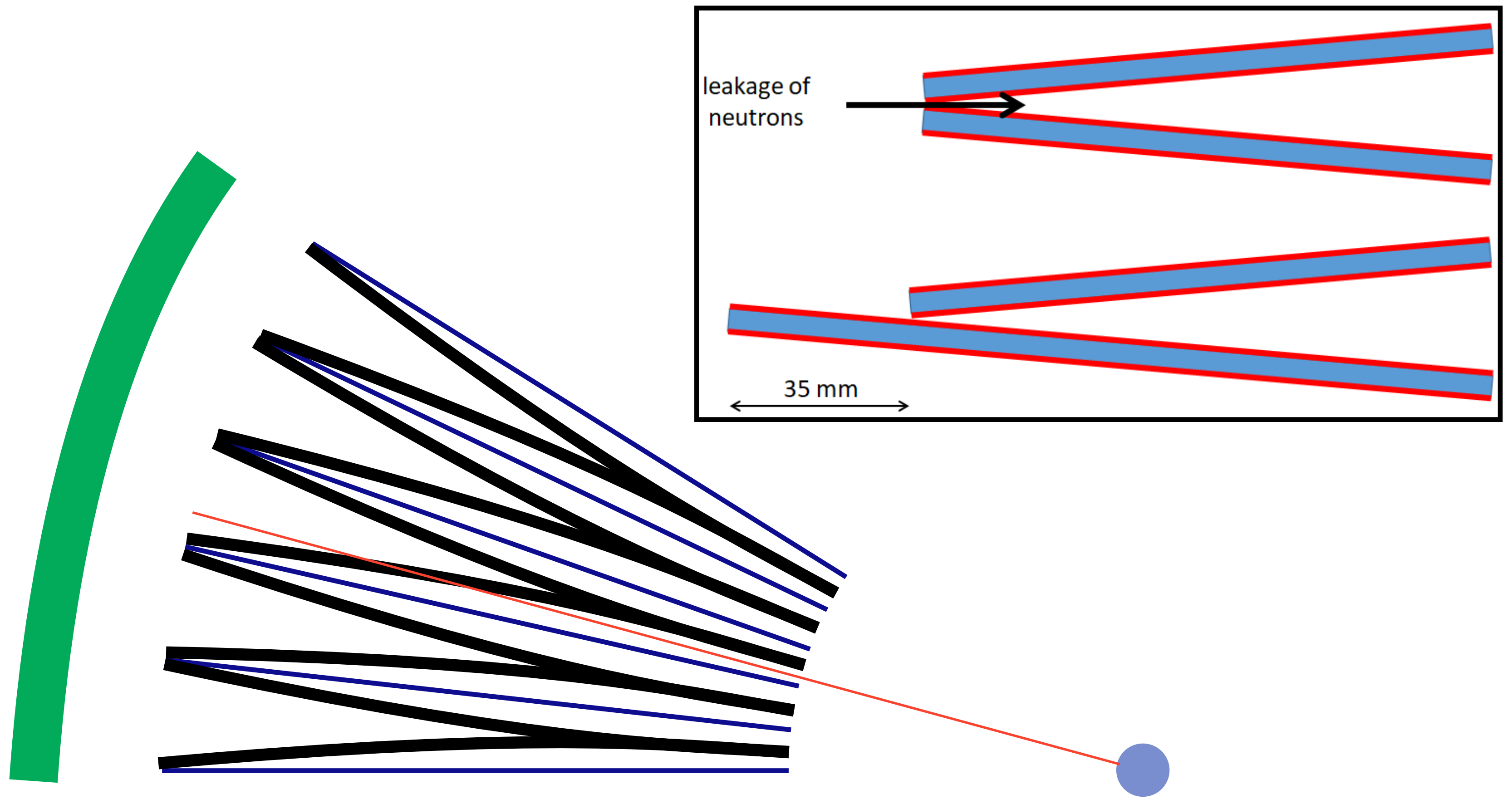
Science and Technology Facilities Council



WISH: analyzer

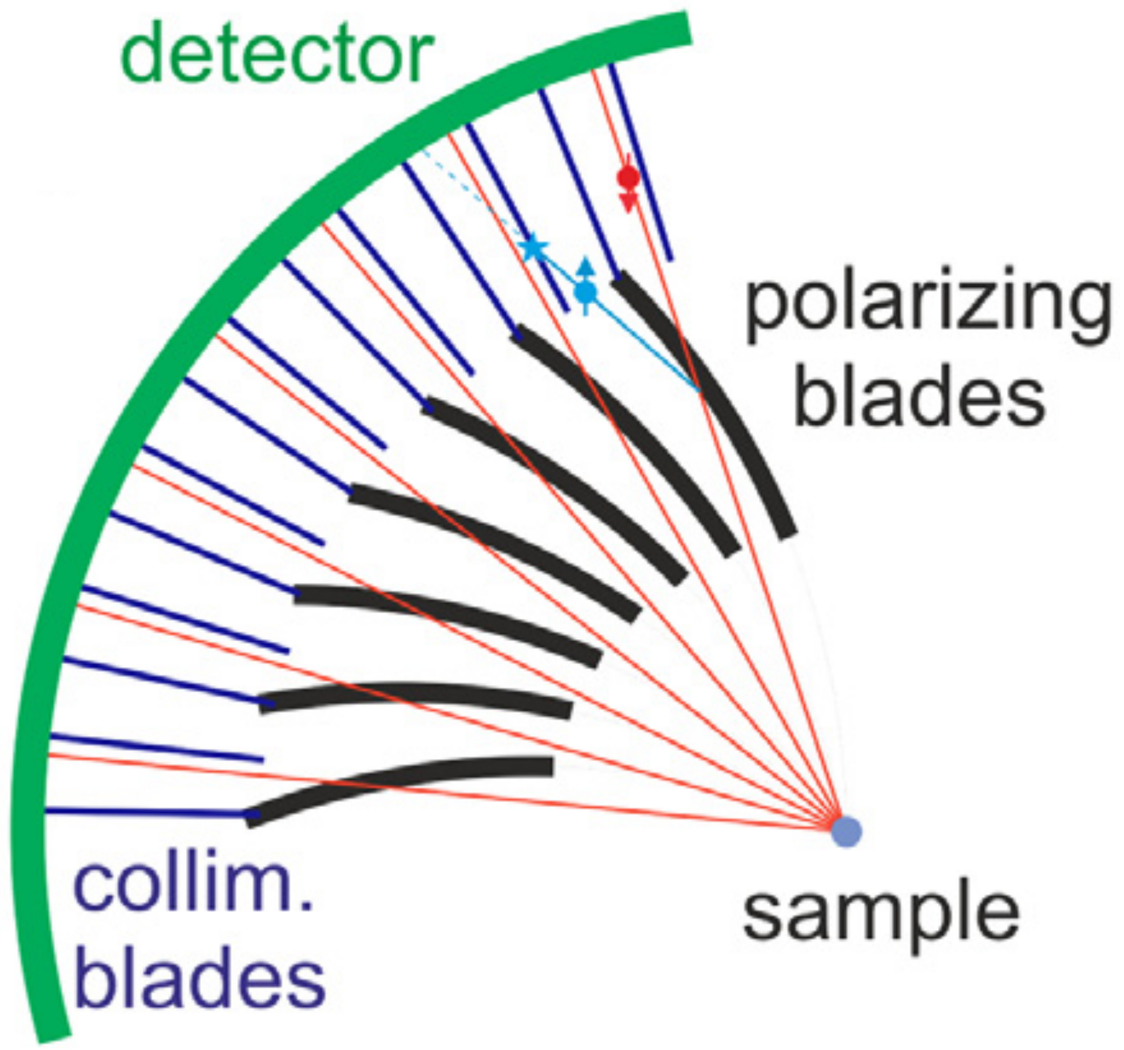
- Use transmission rather than reflection to improve cost, transmission, corrections:

V-cavity



+ fewer channels
- mirror overlap
- sample environment spurions

Z-cavity



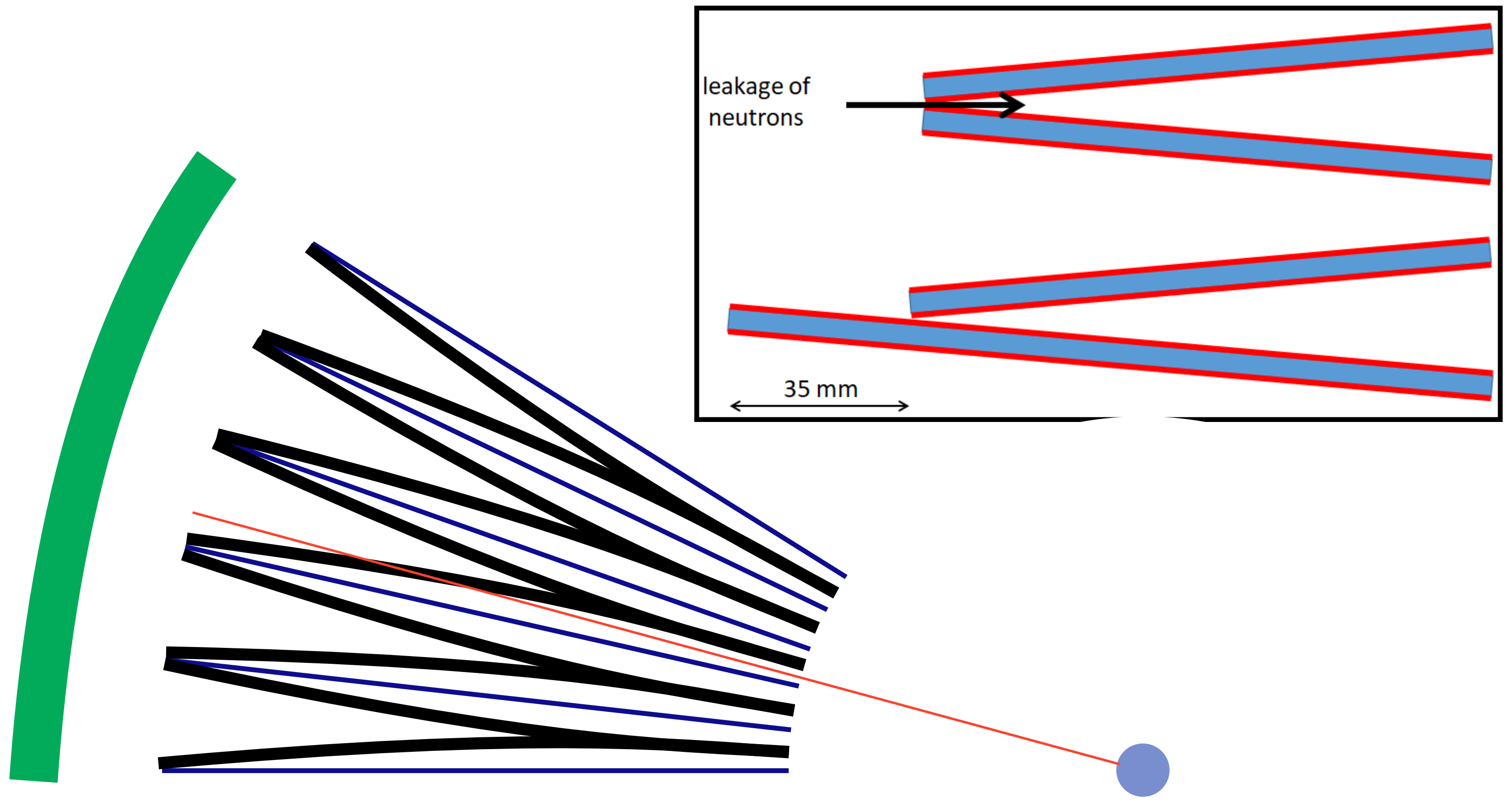
+ more flexible collimation
- more channels
- crosstalk?

Böni *et al.*, *NIMA* **966**, 163858 (2020)

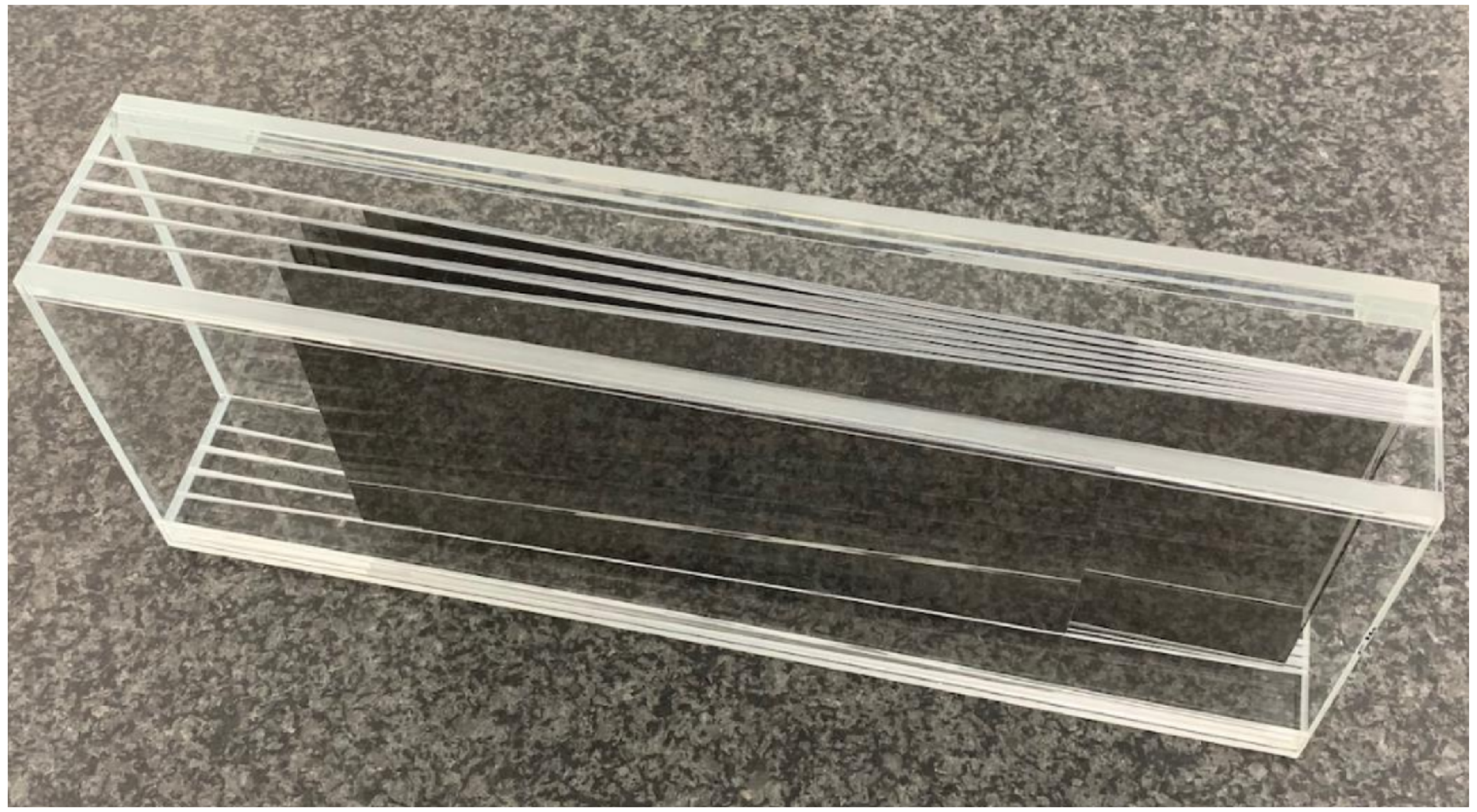
WISH: analyzer

- Three-channel prototype (Swiss Neutronics AG - Michael Schneider, Peter Böni):

V-cavity



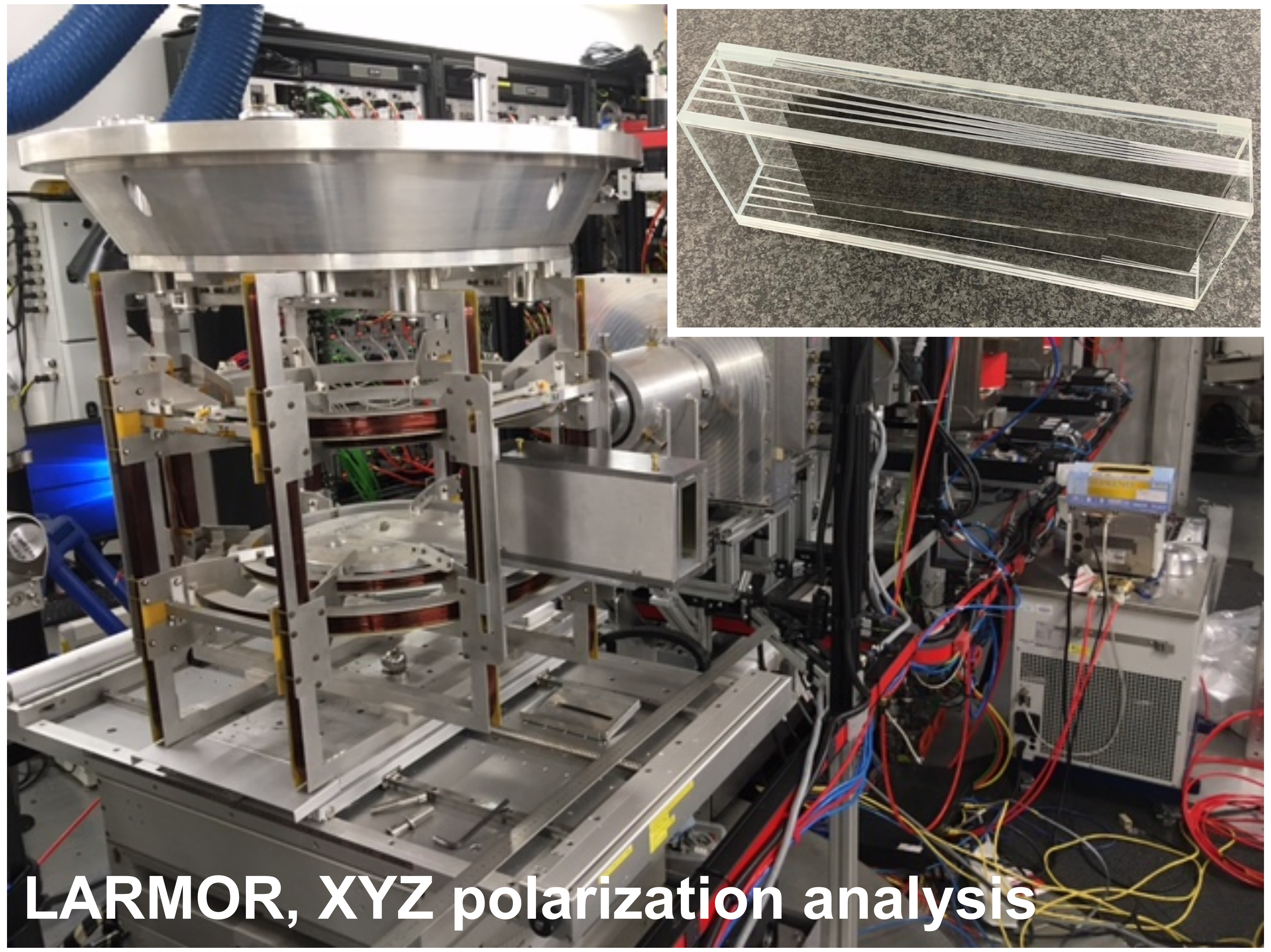
+ fewer channels
- mirror overlap
- sample environment spurions

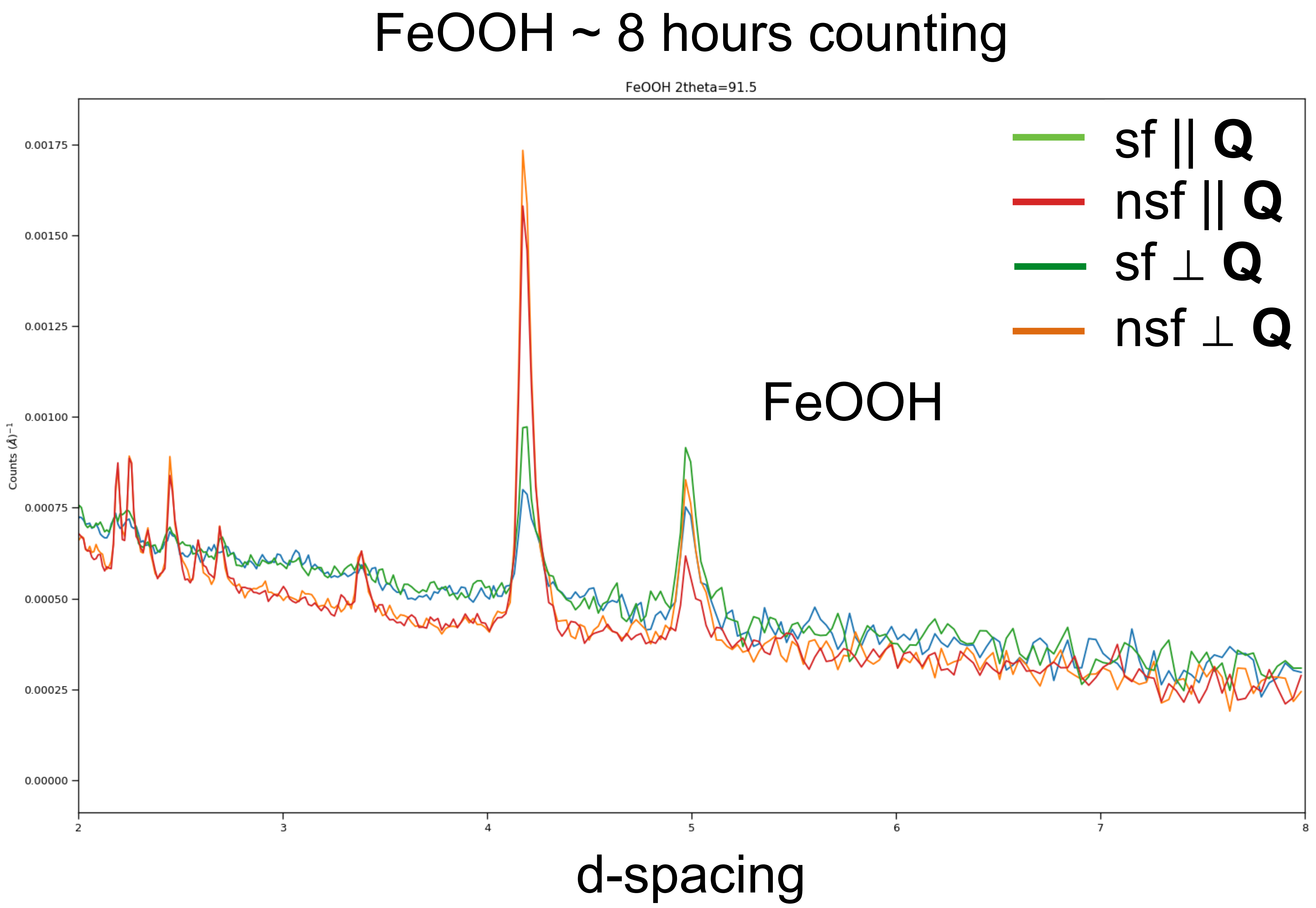


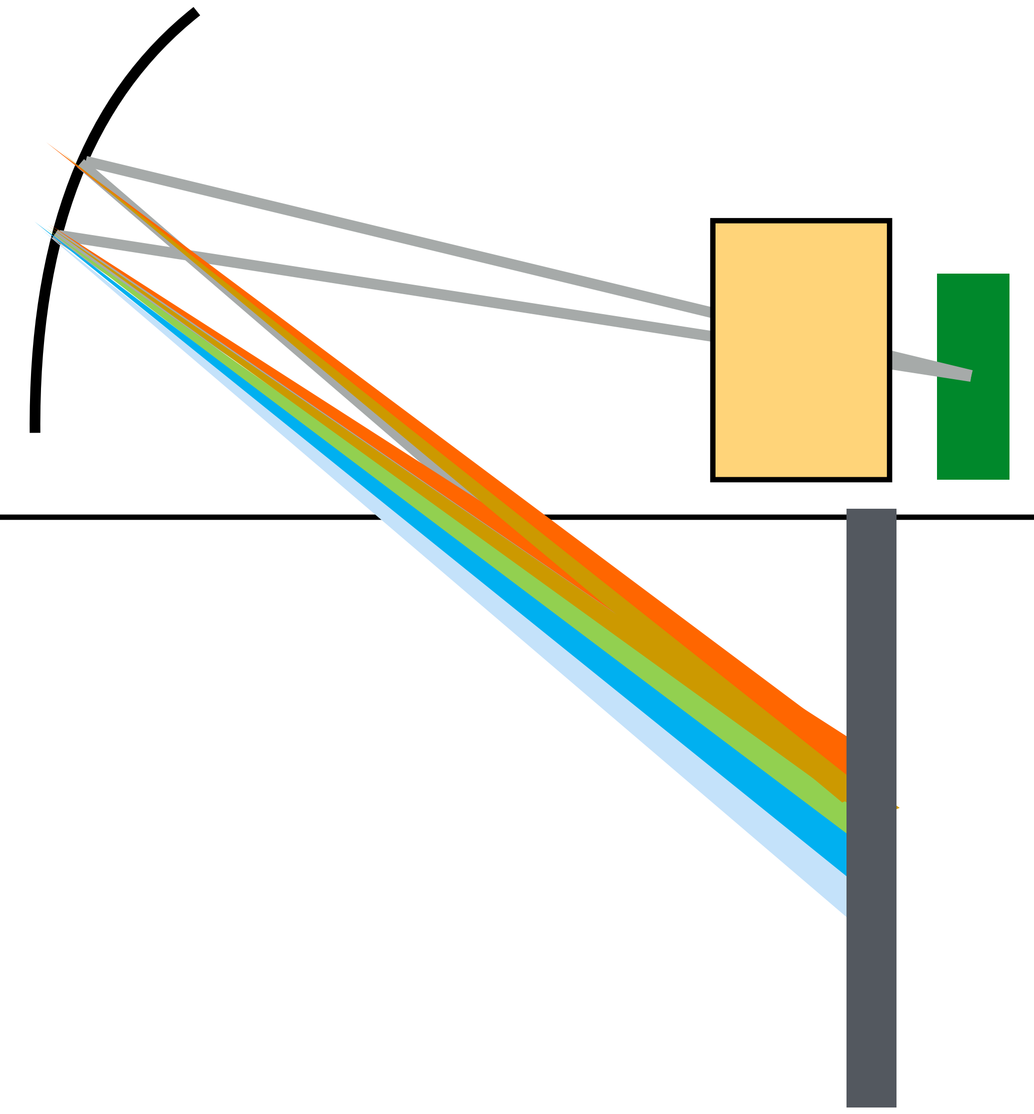
r_{in} = 0.215m, r_{out} = 0.475m, m = 4.5
(λ_{min} = 3.14Å for sample d = 6mm)

Supermirror prototype

- Prototype tested on Larmor instrument - p ~ 96%. Full device (~60°) in production…

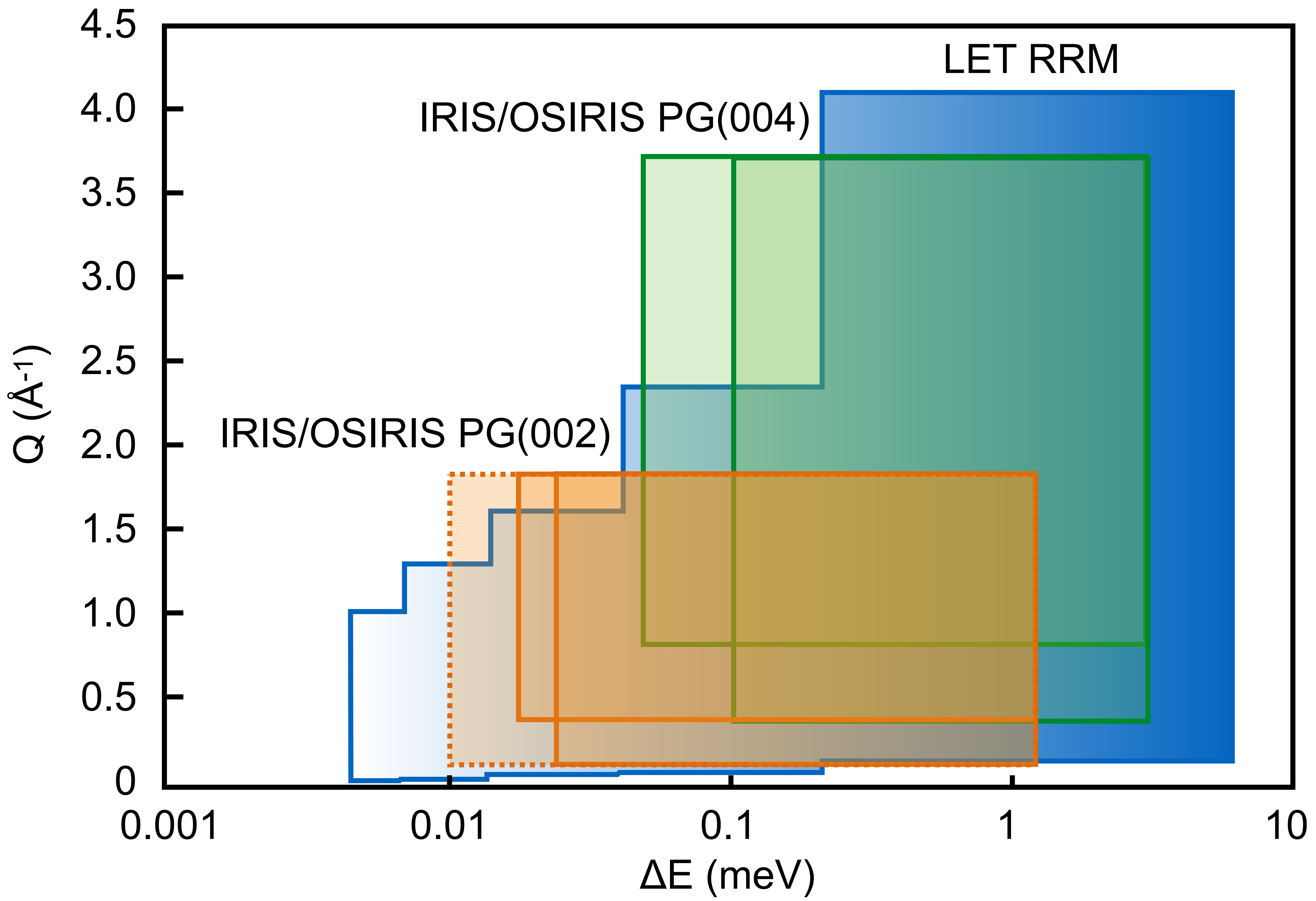






Future: Simultaneous high resolution and high count rate ZPA on SHERPA

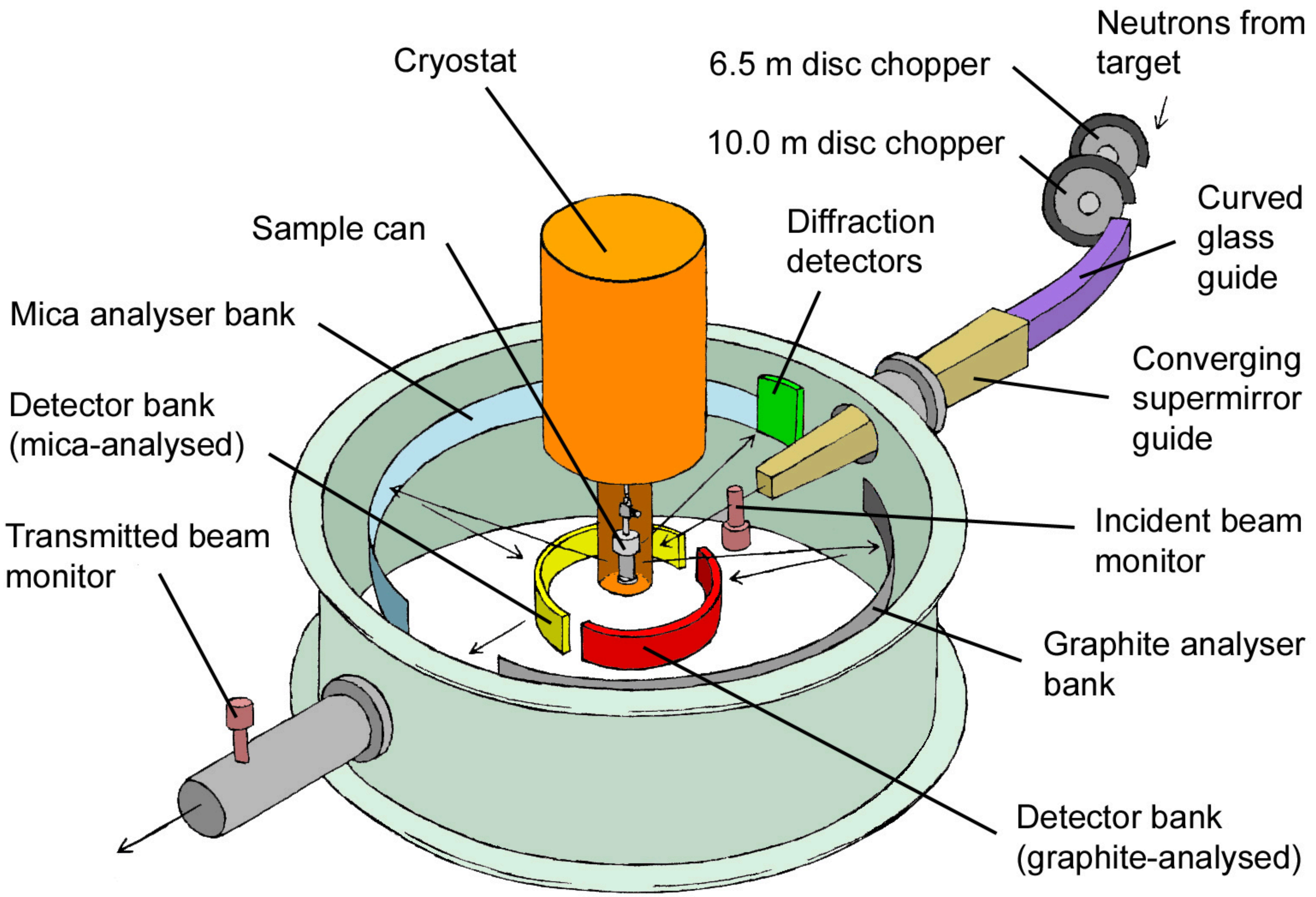
Cold spectrometers at ISIS



- LET (2010)
  - Direct geometry TOF
  - Polarized mode (2019)
- OSIRIS (1998)
  - Indirect geometry TOF
  - Analyzer upgrade
    - Si (111), ΔE=11μeV
  - Guide upgrade
    - ~5x flux gain

From IRIS to SHERPA

- IRIS: indirect geometry time-of-flight spectrometer
  - Part of original instrument suite (1988)
  - Workhorse instrument
    - *m* = 1 curved guide
    - *m* = 2 focusing nose
    - L_1 = 36.5 m
    - PG(002) analyzer
    - Resolution ΔE=17.5μeV



Carlile and Adams, Physica B **182**, 431 (1992)

SHERPA: Primary spectrometer

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- Modern double-elliptical supermirror guide (like OSIRIS) → **Gain x10**

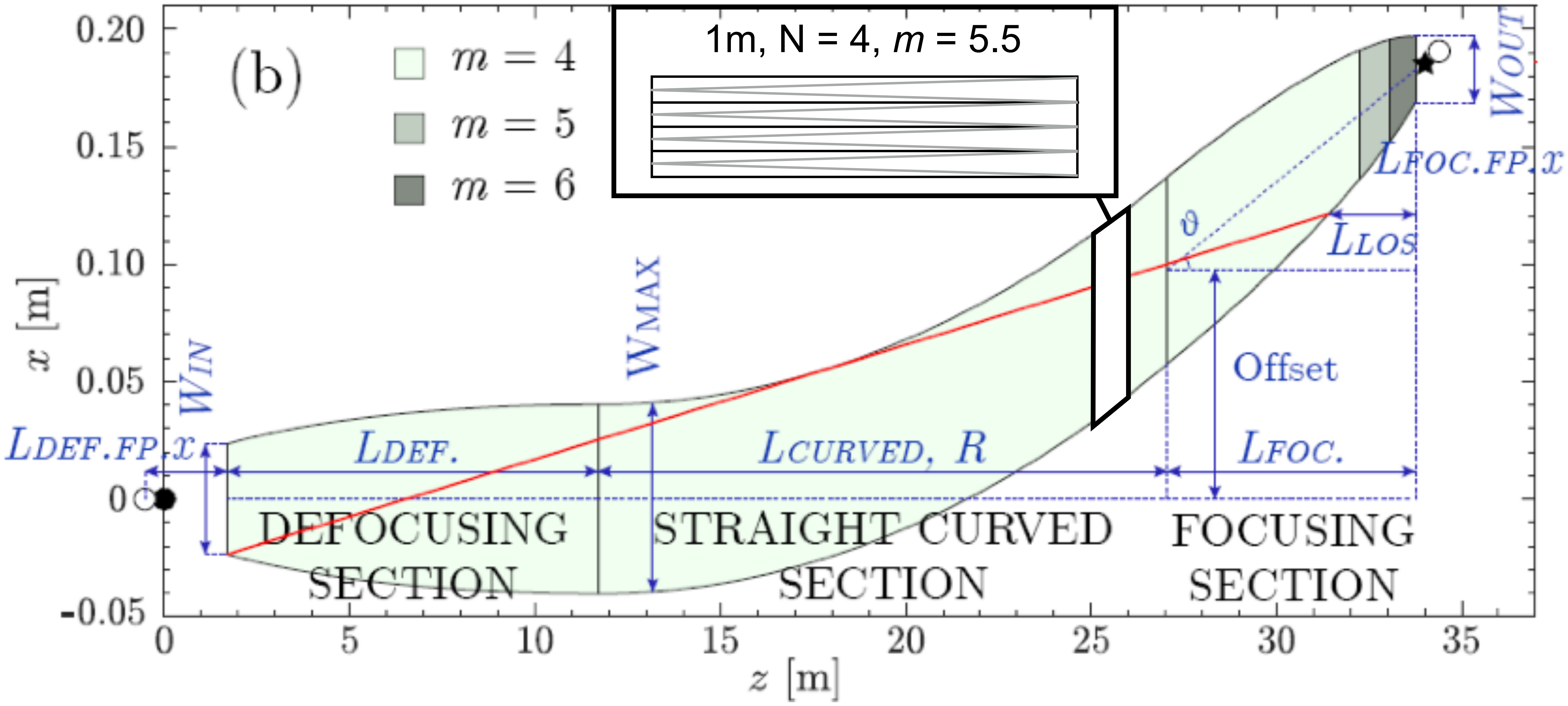
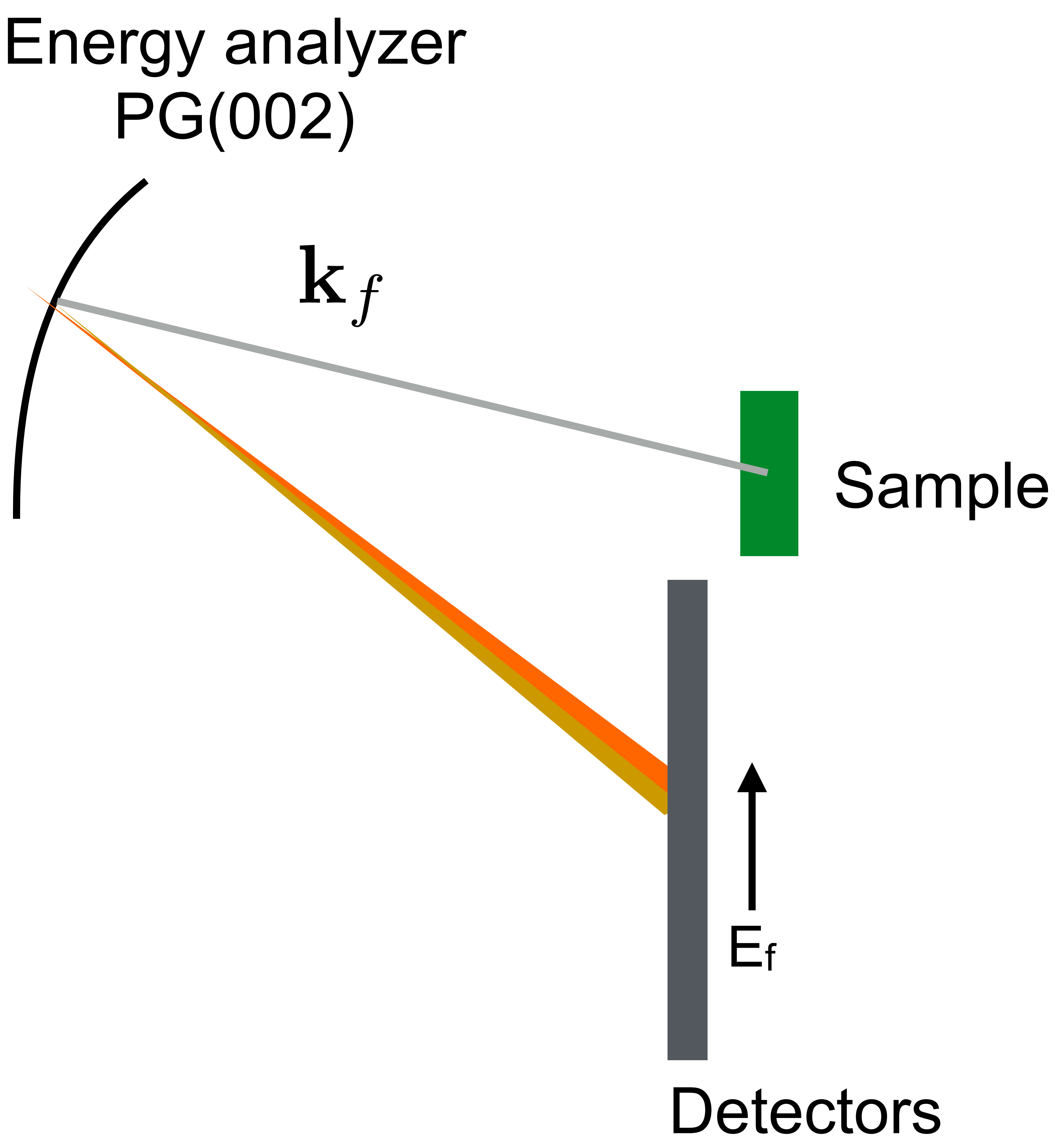


Figure: A. Perrichon and F. Demmel

SHERPA: Secondary spectrometer



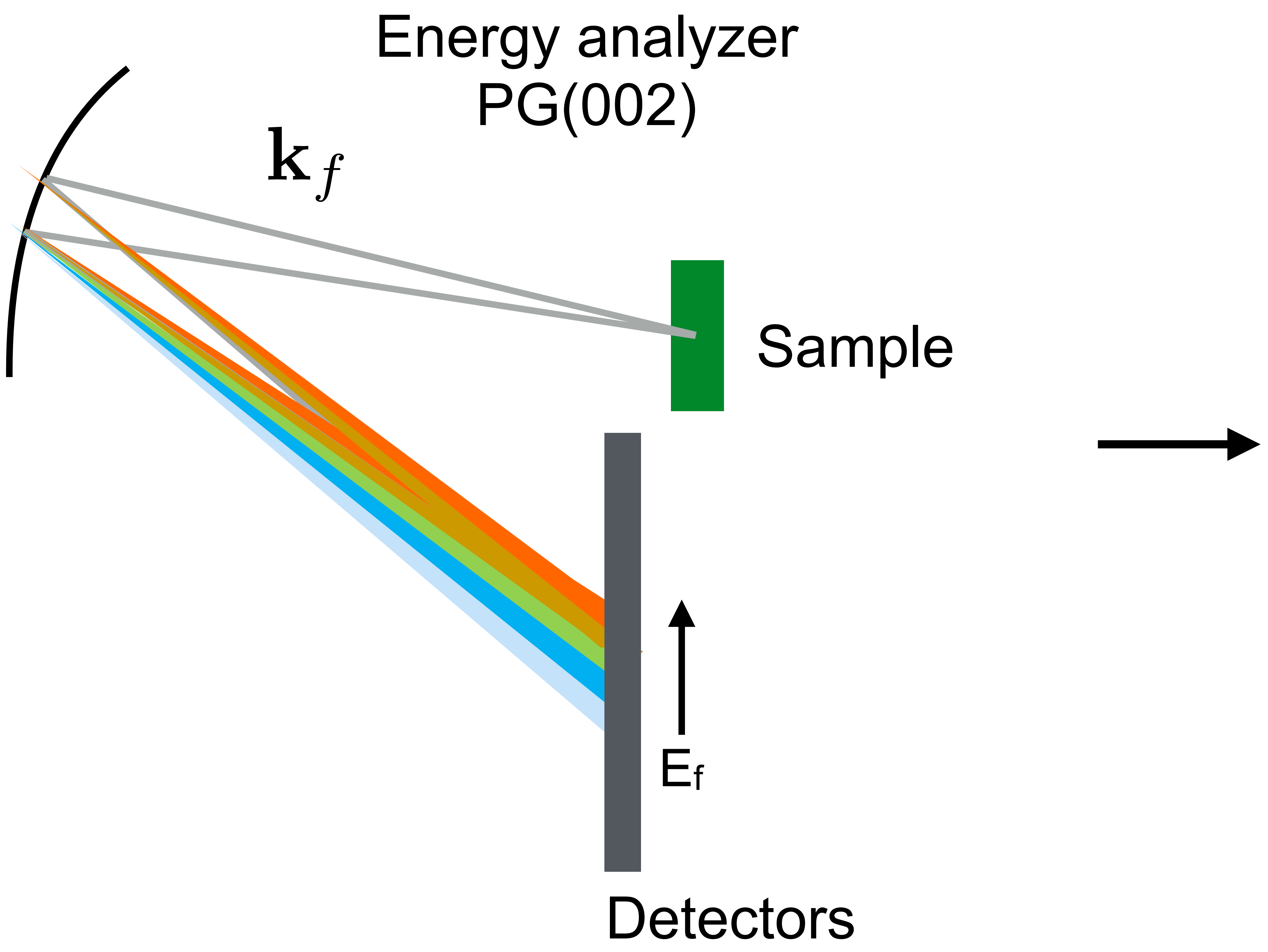
$$I \propto \Phi d\Omega \Delta\lambda$$

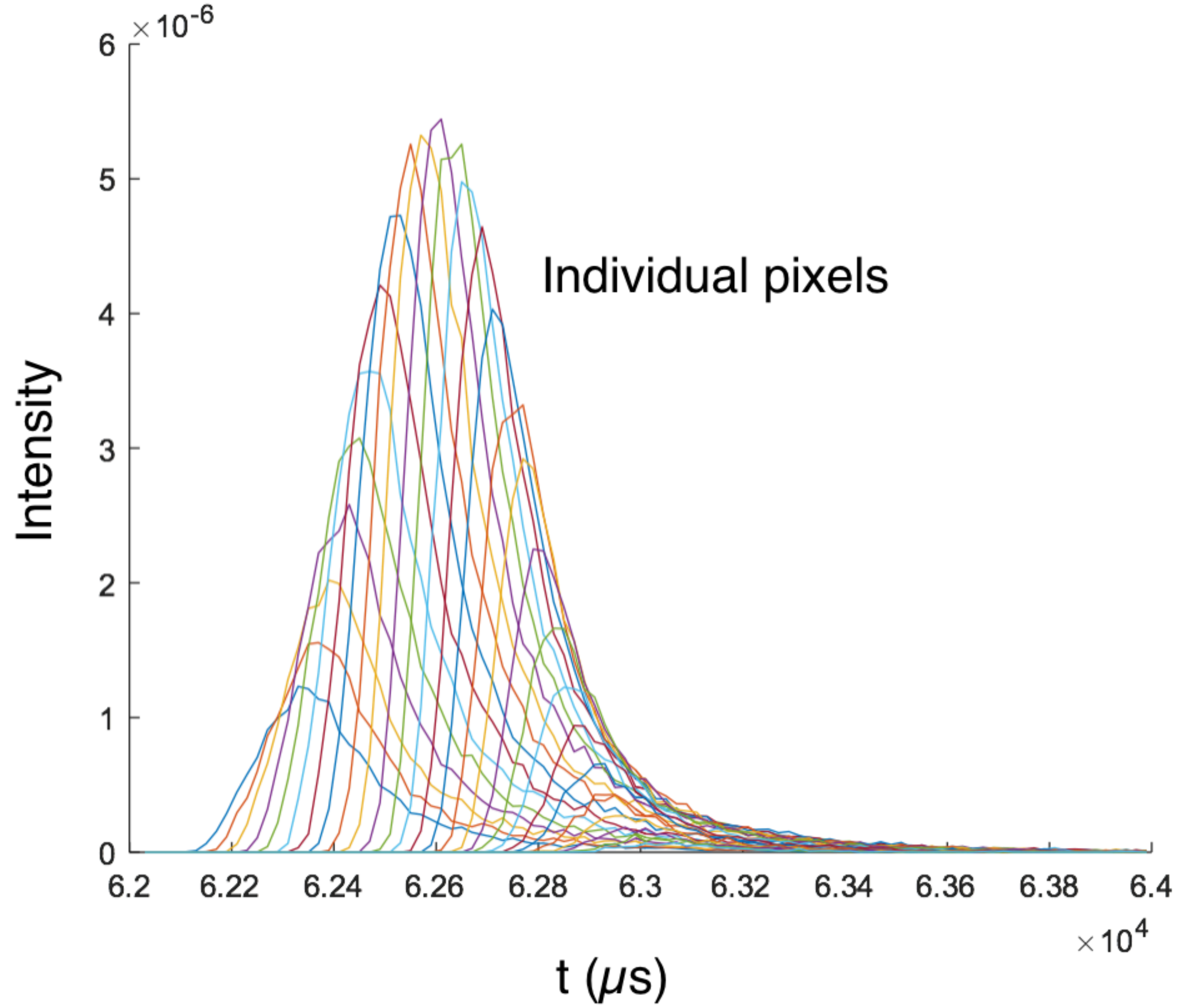
$$\Delta\lambda = \mu\lambda \cot\theta$$

	λ (Å)	μ(°)	cot θ	dΩ	Φ	**Gain**
IRIS	6.64	0.8	0.0437	0.2	1E+07	**1**
SHERPA	6.47	1.5	0.2586	0.6	1E+08	**330**

SHERPA: Secondary spectrometer

- Use prismatic effect in secondary spectrometer





R. Bewley, Rev. Sci. Instrum. **90**, 075106 (2019)

SHERPA: Secondary spectrometer

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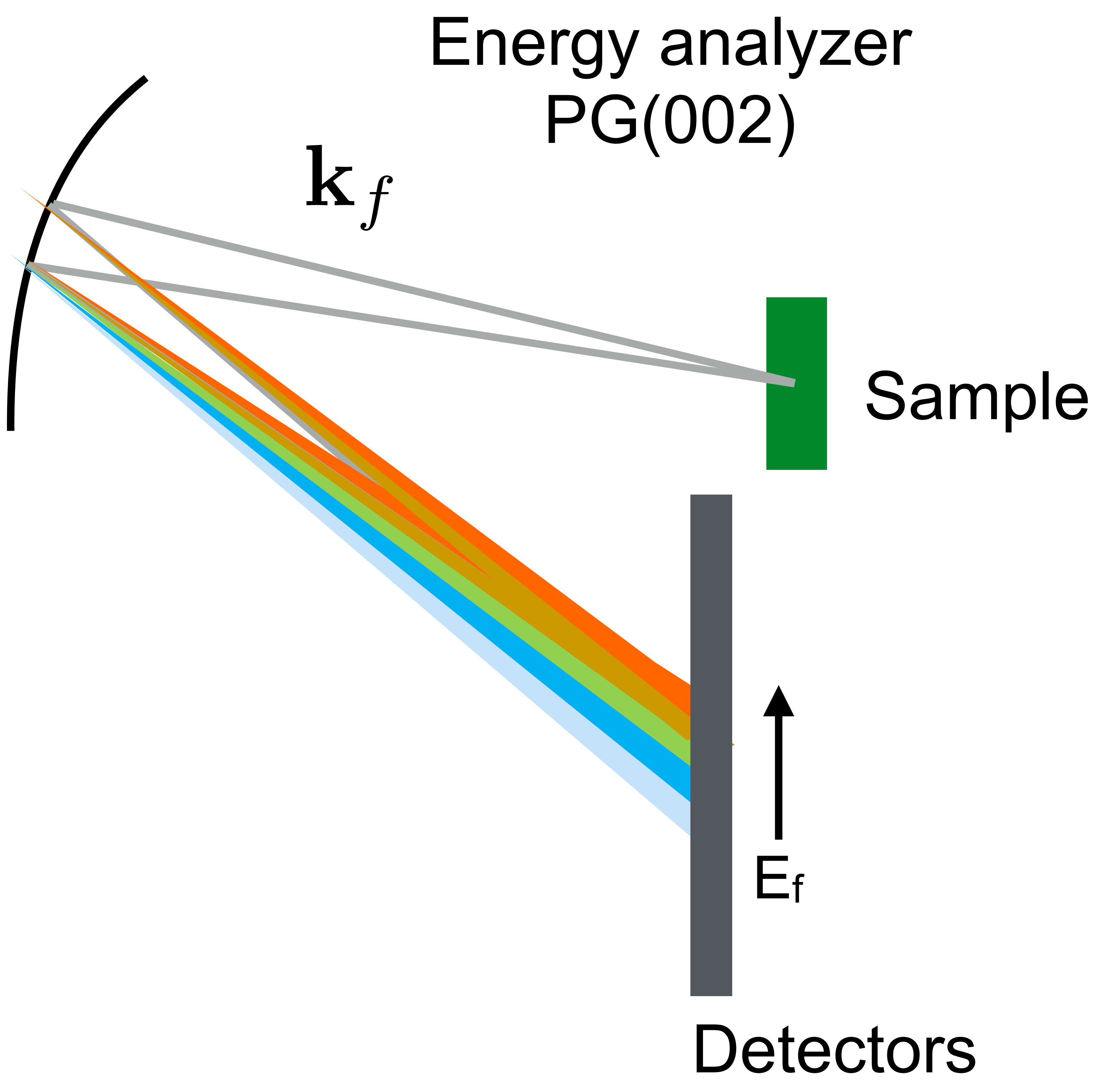
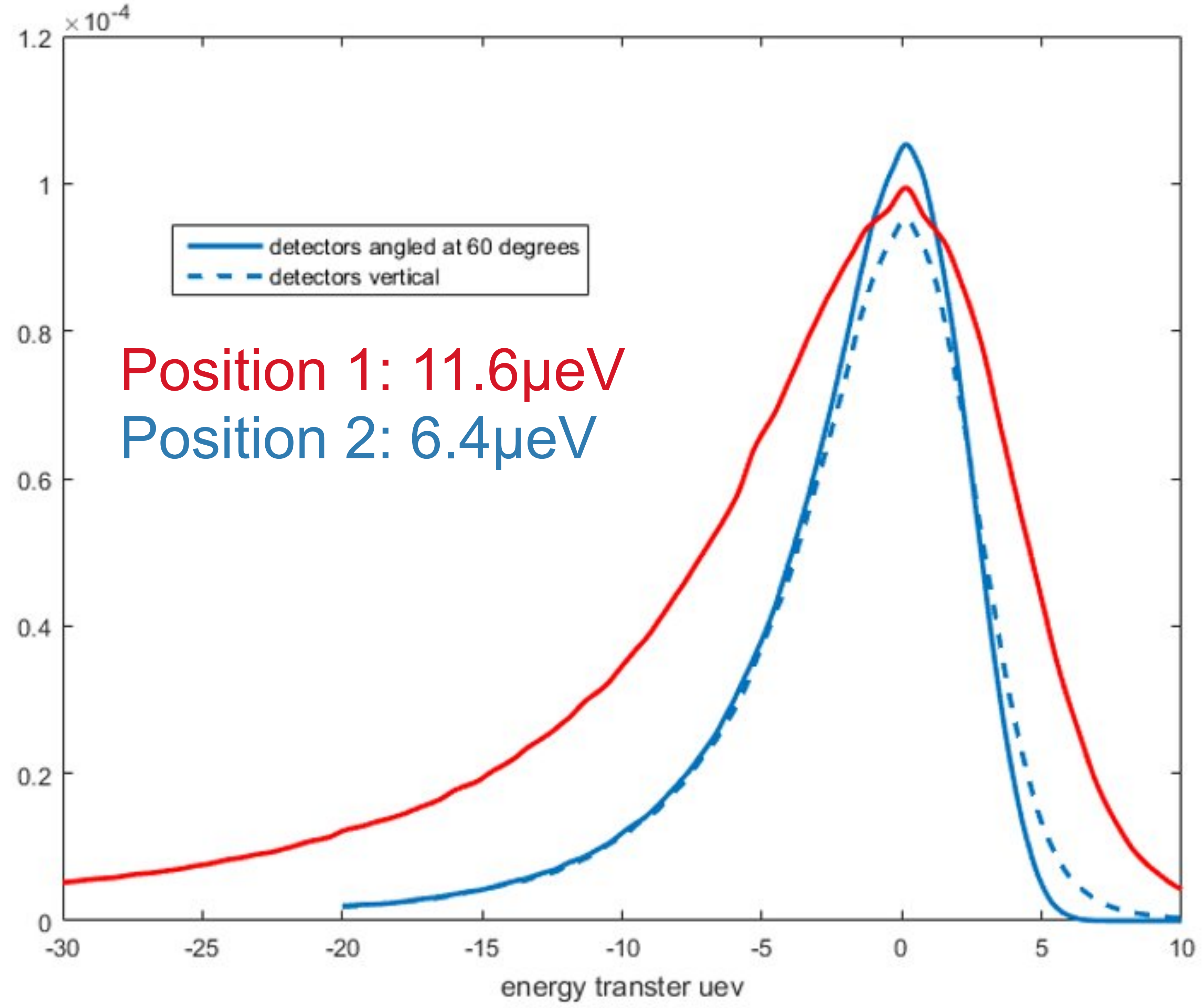
- Use prismatic effect in secondary spectrometer

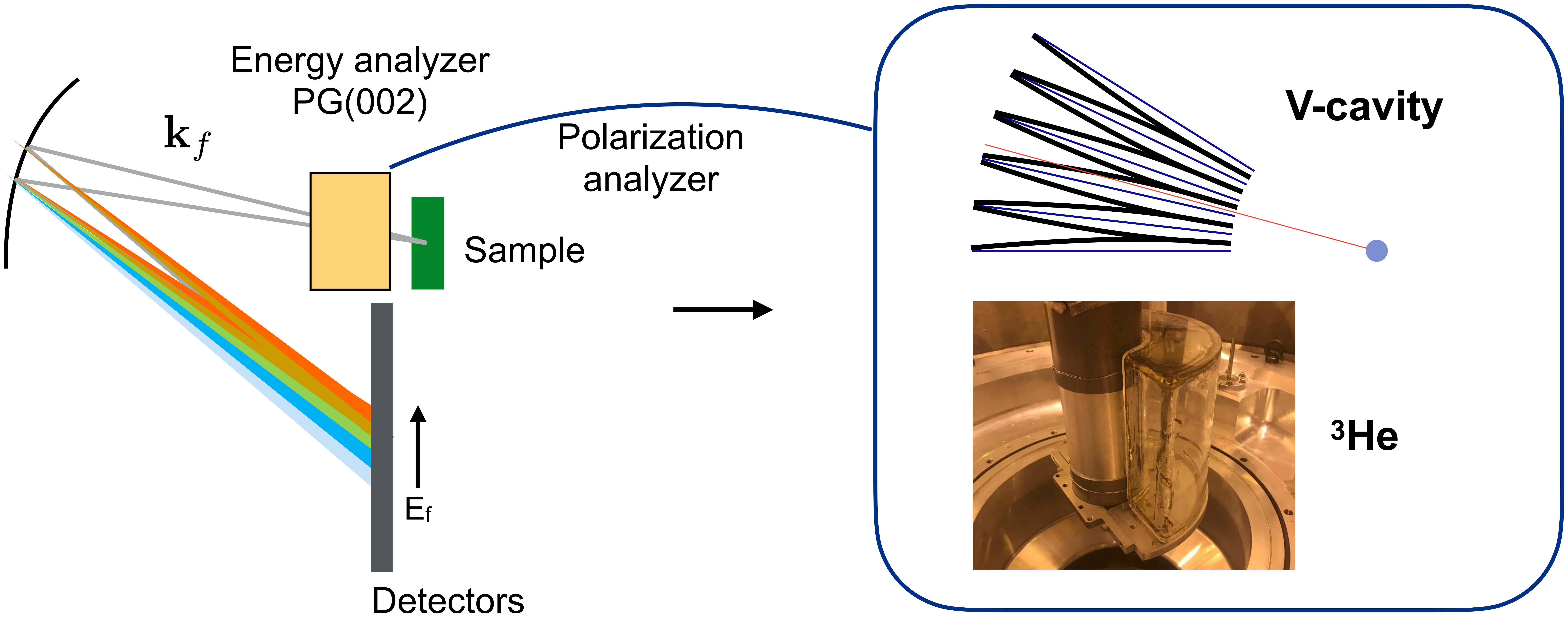




R. Bewley, Rev. Sci. Instrum. **90**, 075106 (2019)

SHERPA: Secondary spectrometer

- Polarization analyser: V-cavity or ^{3}He cell?



R. Bewley, Rev. Sci. Instrum. **90**, 075106 (2019)

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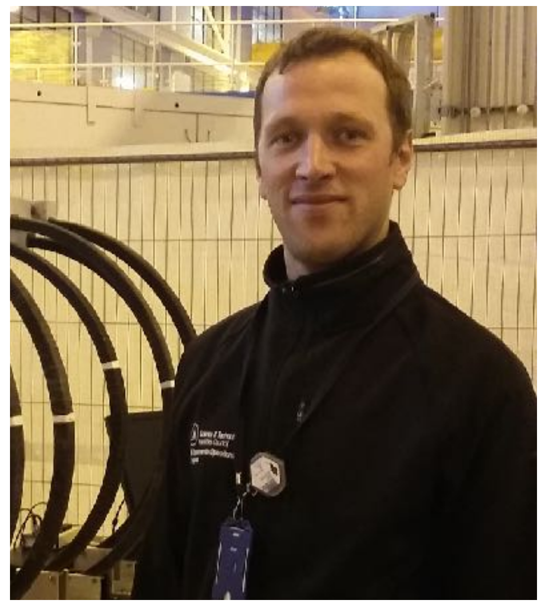

SHERPA Project
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