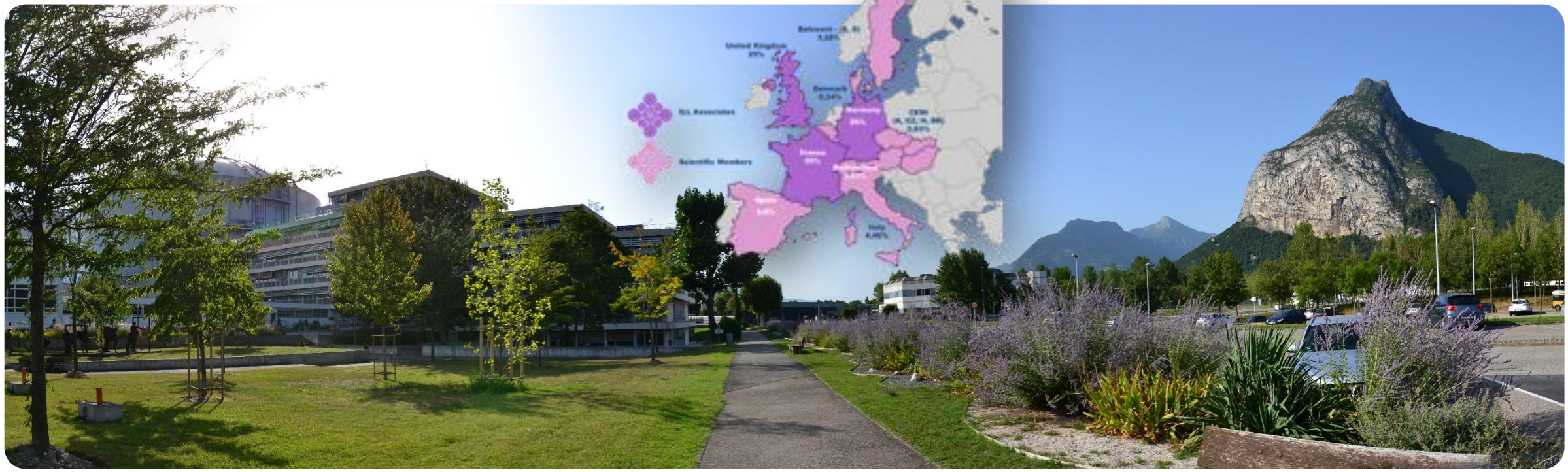
Institut Laue-Langevin : 50 years at the service of science

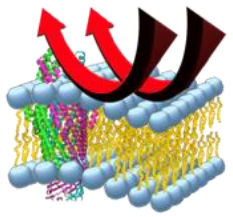


Giovanna Fragneto

Large Scale Structures group leader

Head of Soft Matter Science and Support

Chair *Grands Instruments Européens* Université Grenoble Alpes



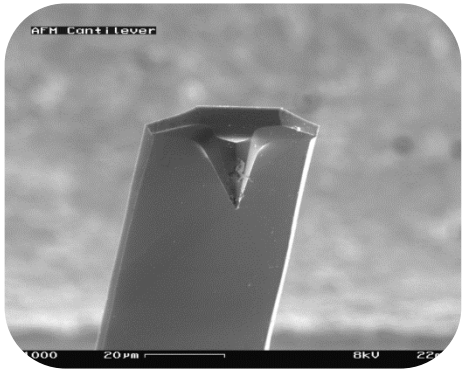
Grenoble has a very high Concentration of Scientific Infrastructure

The EPN Campus in Grenoble hosting EMBL, ESRF, IBS and ILL
Partnerships among the institutes notably PSB and PSCM

MATERIALS EXPLORATION LEANS ON VARIOUS SOPHISTICATED TOOLS

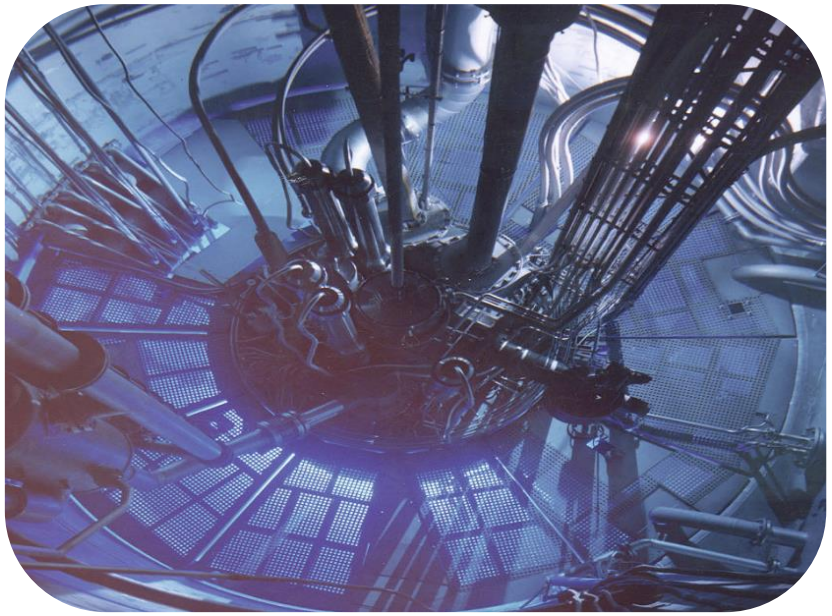
Europe has the world's leading infrastructure for characterizing materials.

Microscopy



Nuclear Magnetic Resonance

Neutron scattering



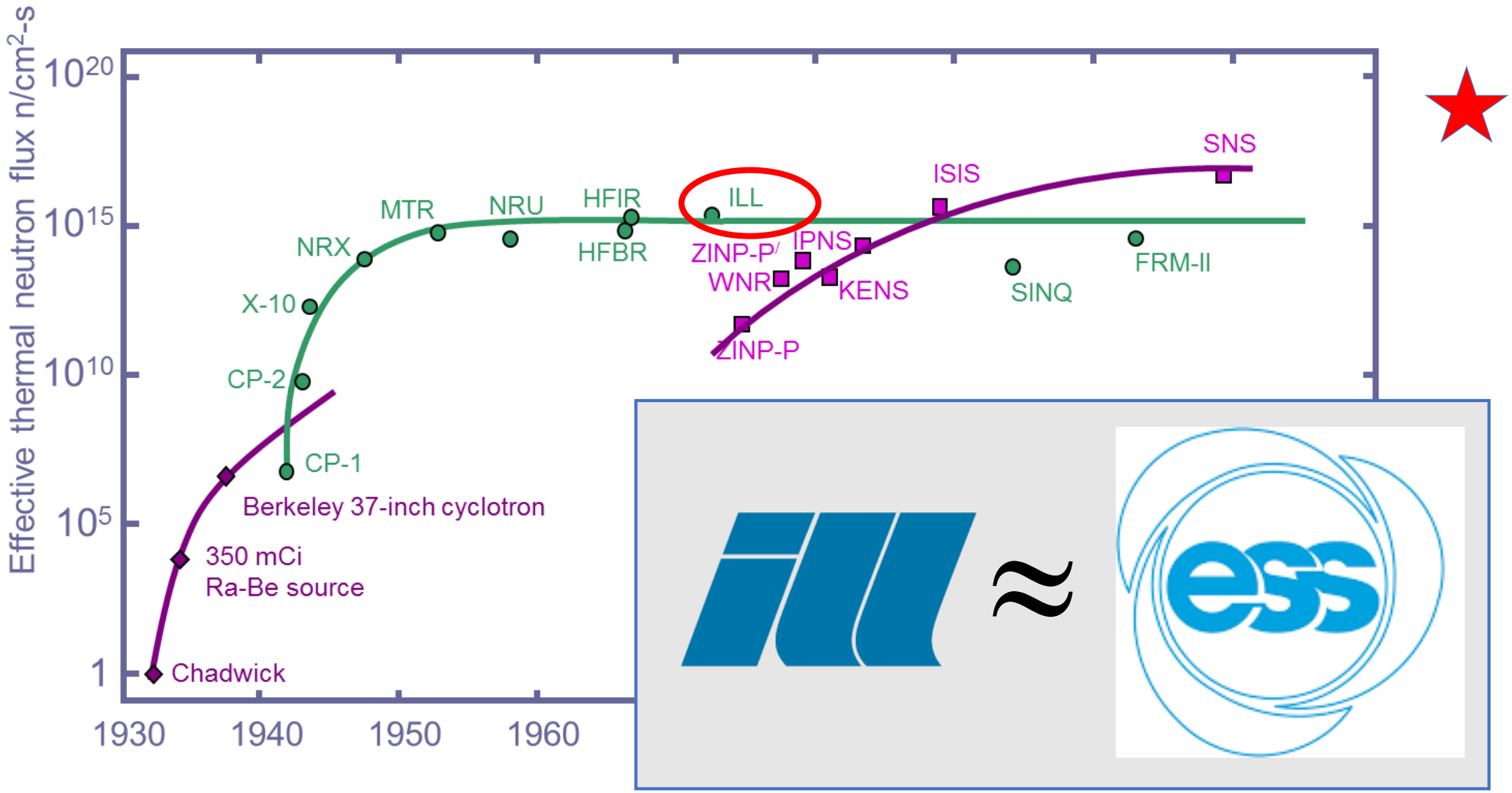
Synchrotron radiation

Daily Telegraph

EUROPE ENJOYS A VERSATILE AND BROAD NETWORK OF NEUTRON SOURCES

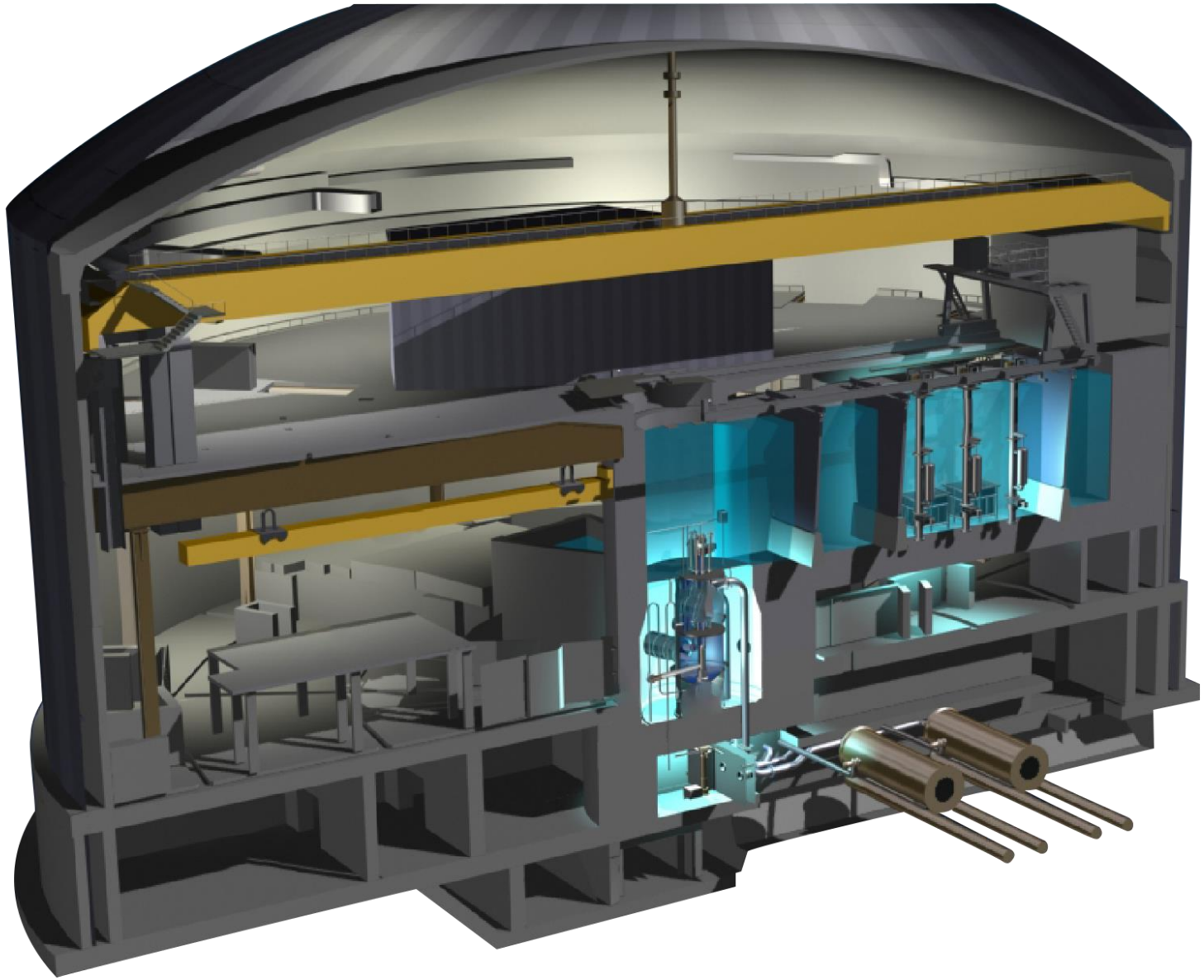
The neutron is a unique and irreplaceable probe,
with characteristics that cannot be supplanted by other methods.

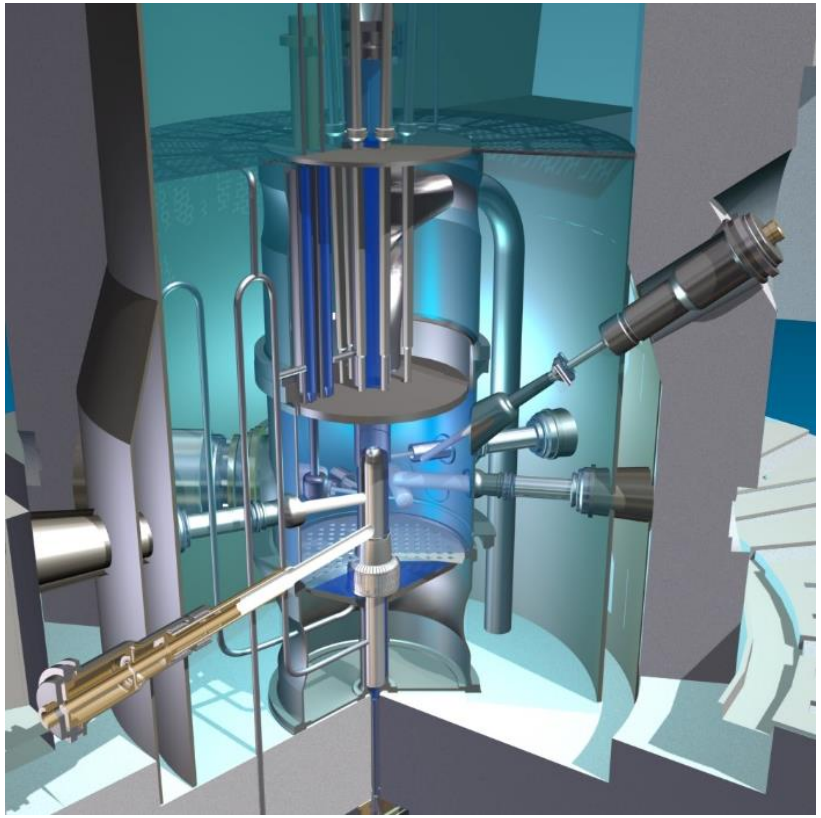
ILL : a remarkable reactor



(Updated from *Neutron Scattering*, K. Skold and D. L. Price, eds., Academic Press, 1986)

The ILL Reactor



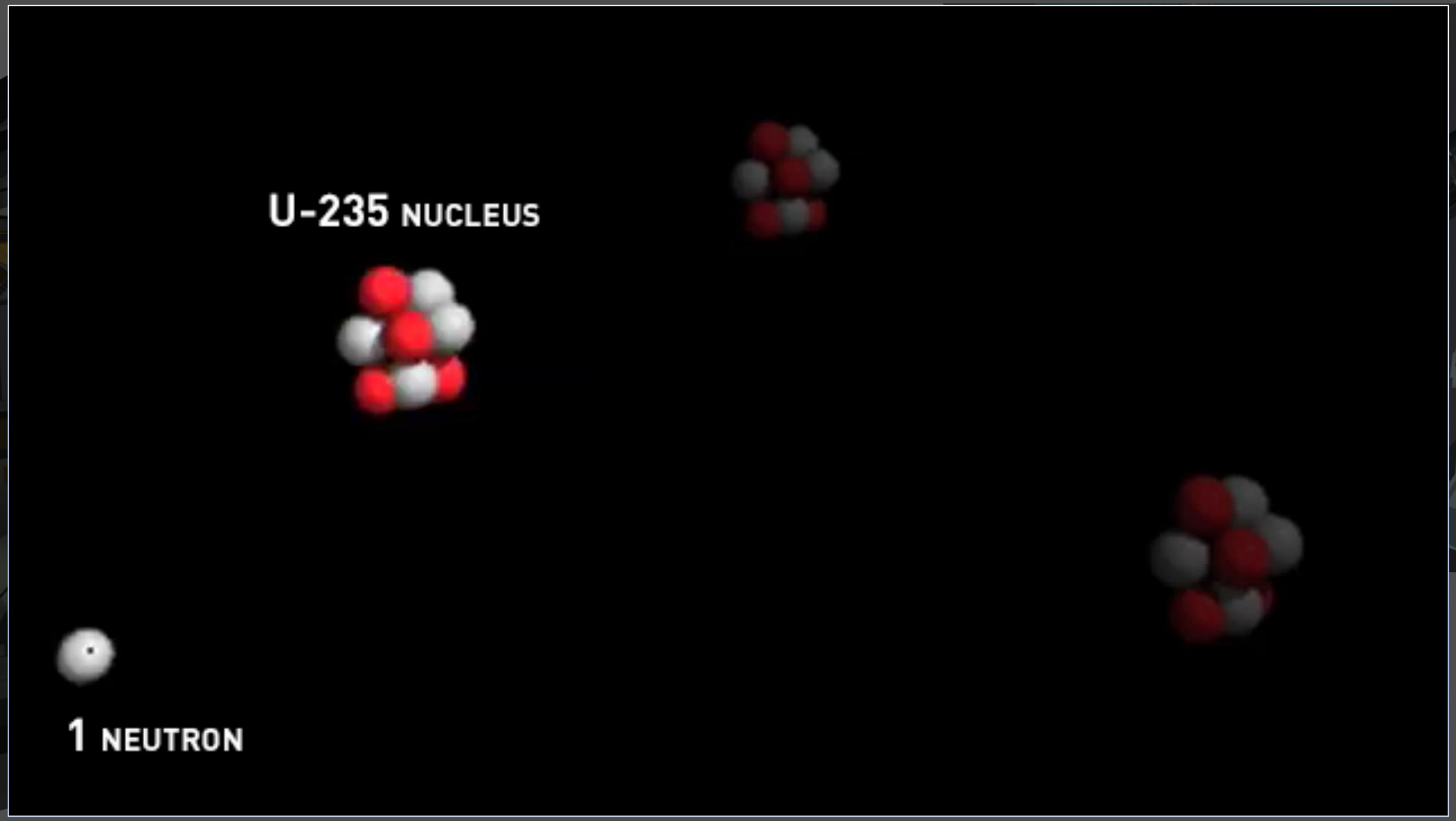


A neutron source generating

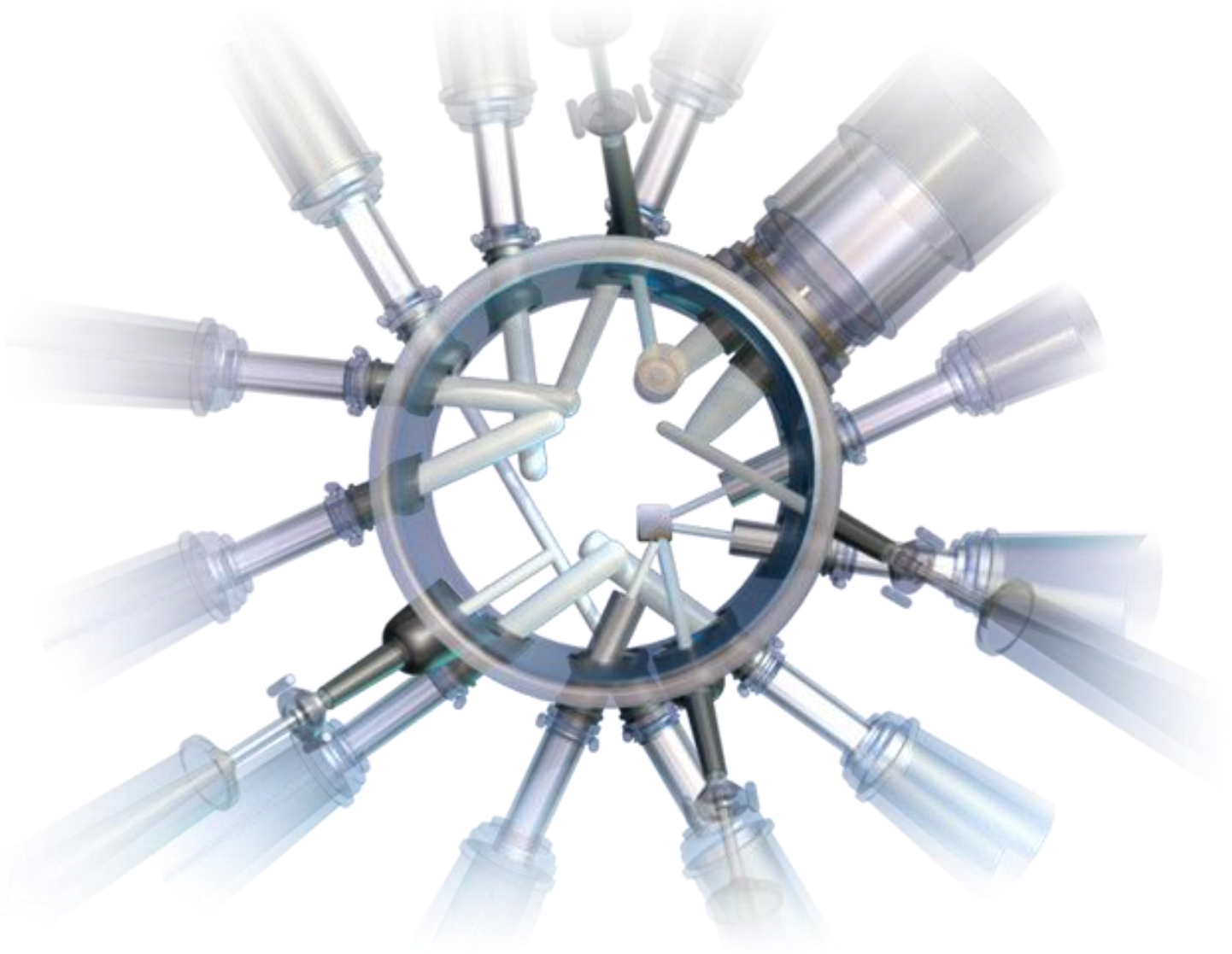
5 x 10^{18} fast neutrons/sec

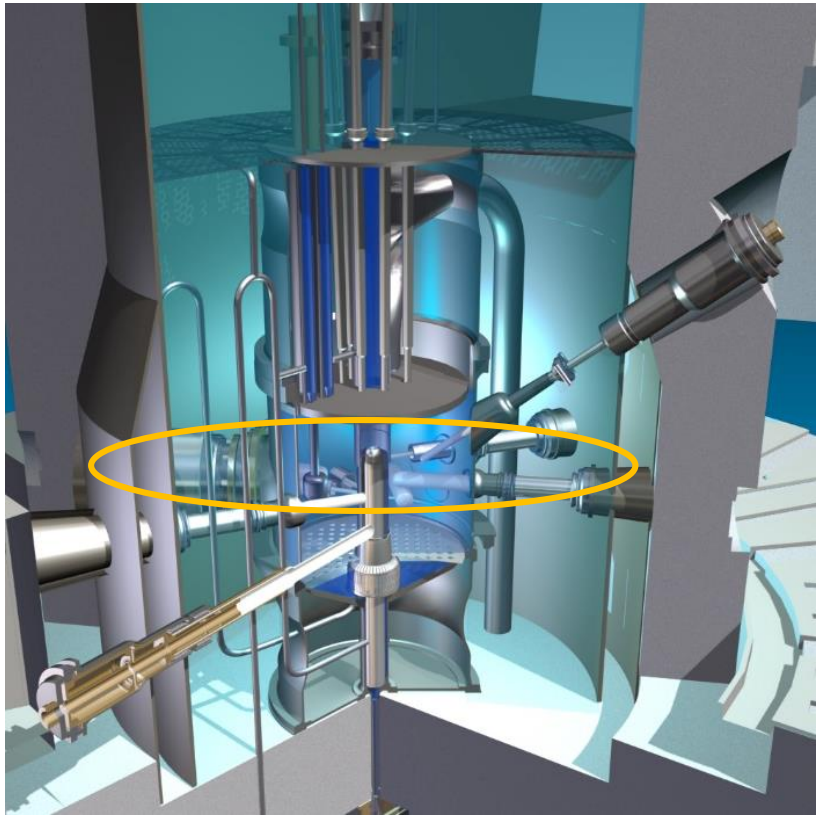
at a max power of 58 MW

Neutrons production by controlled chain reaction

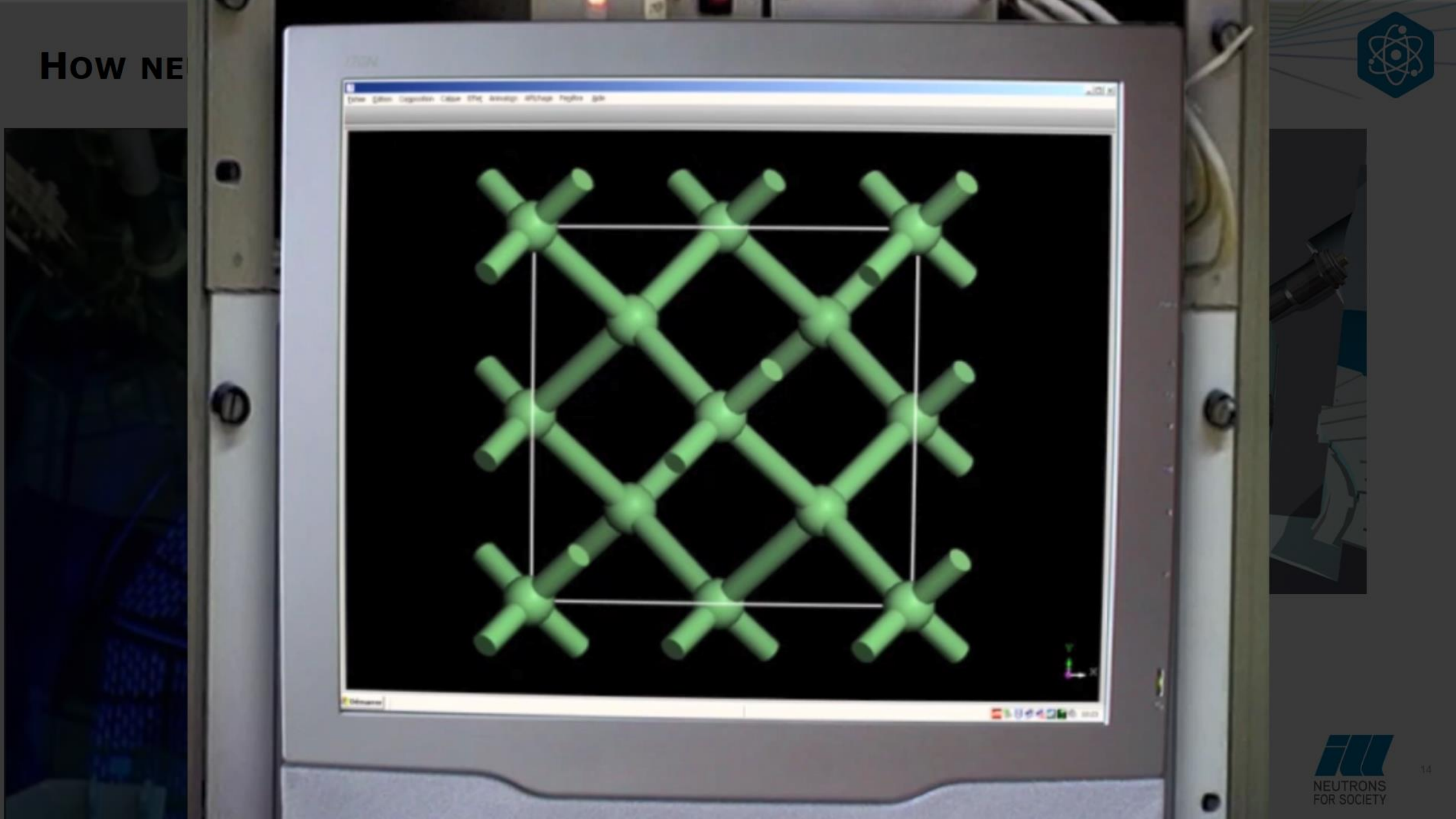


How neutrons are extracted and guided



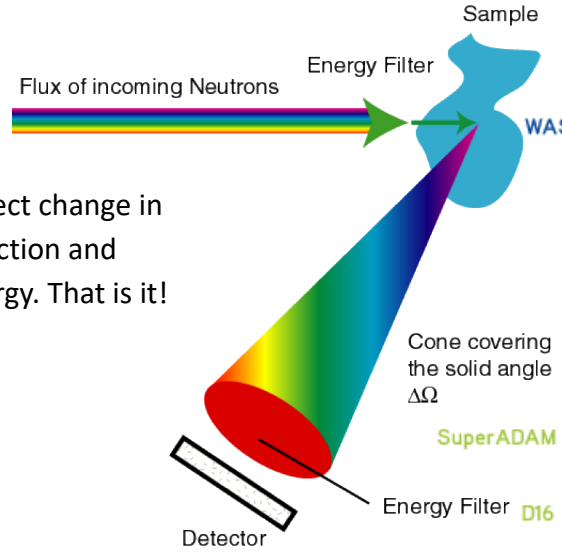


How ne

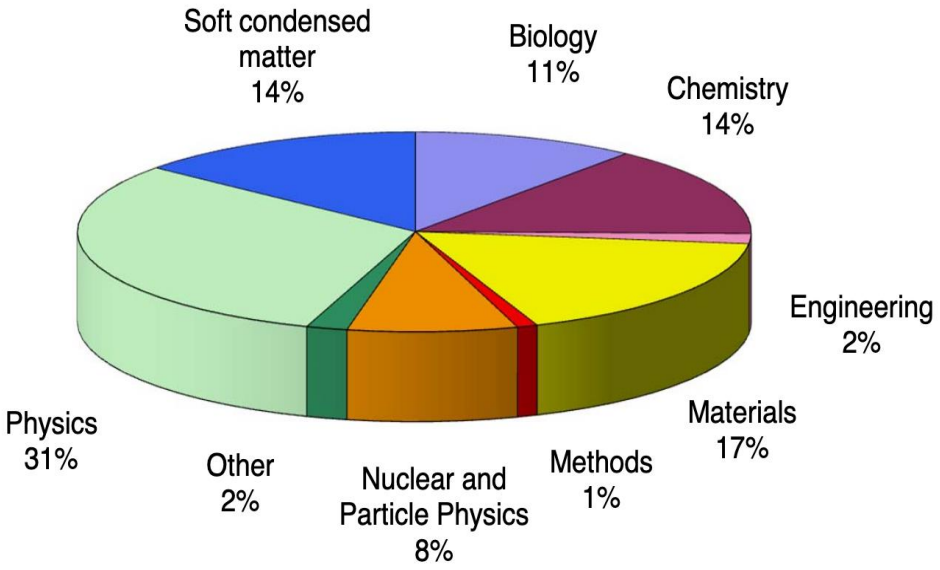


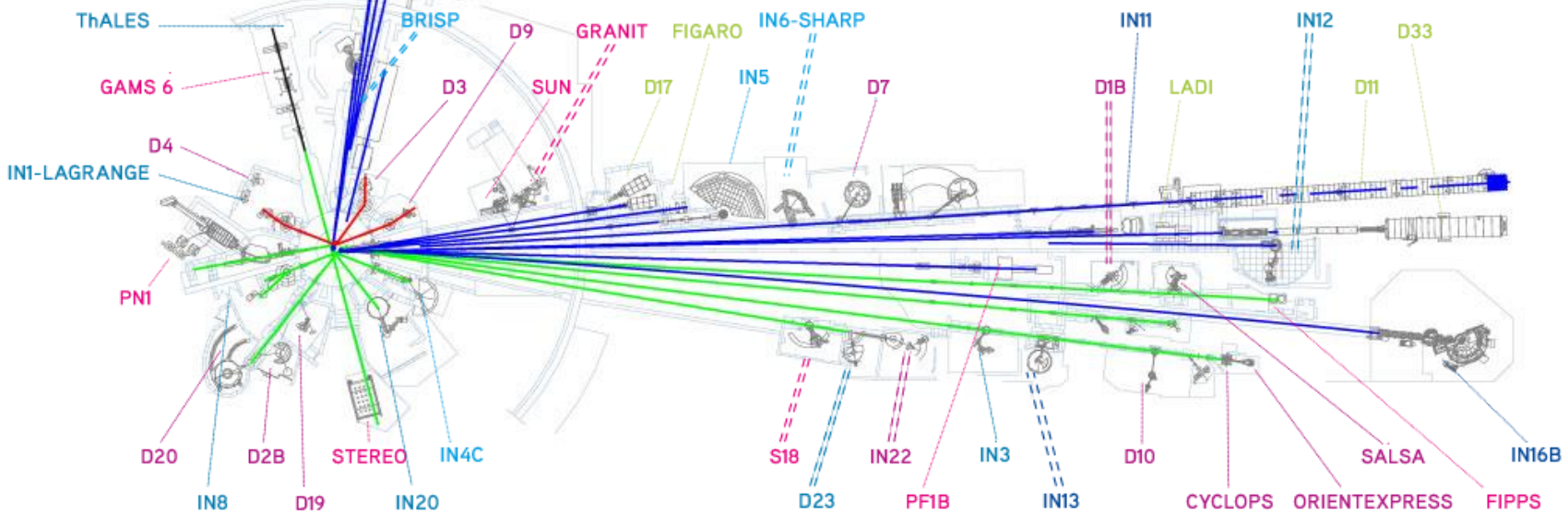
NEUTRONS FOR SOCIETY

The ILL's instrument suite



Detect change in direction and energy. That is it!

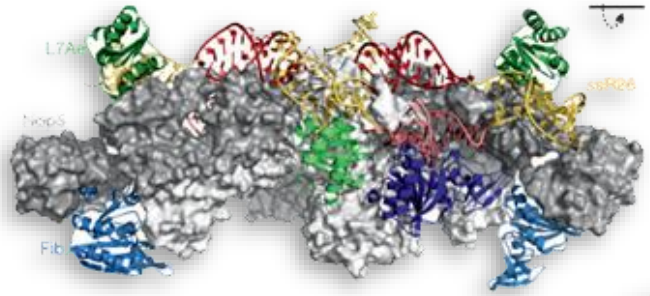


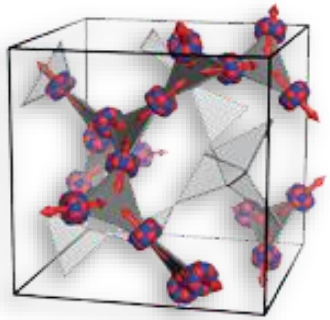


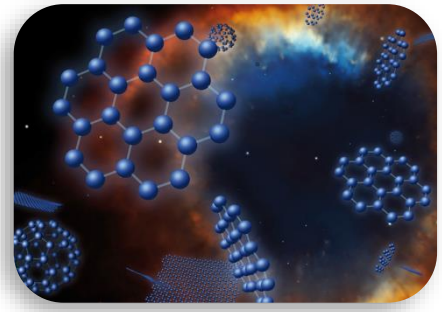
Liquids, gases, solid matters may all be studied with neutrons

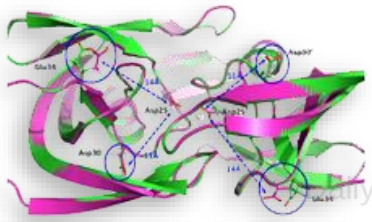
Understanding materials

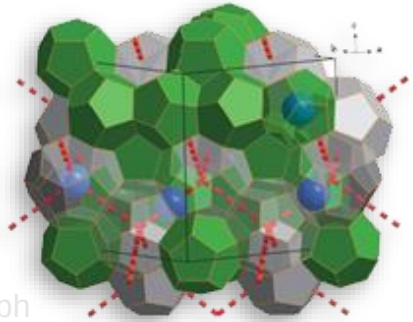
underlies all of modern technology.

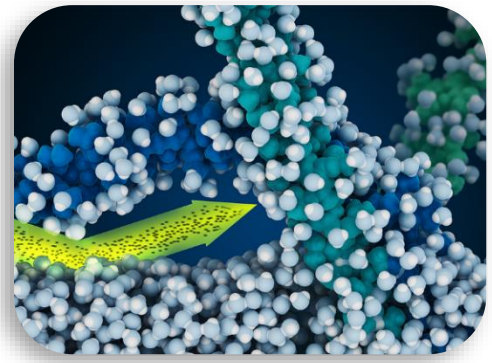


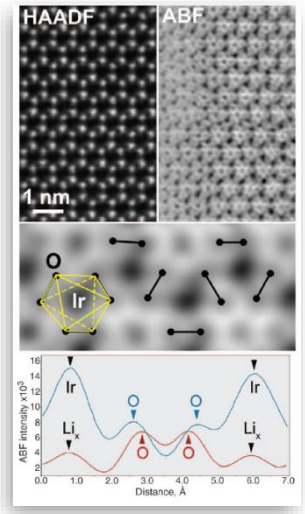


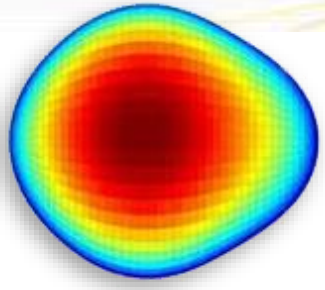


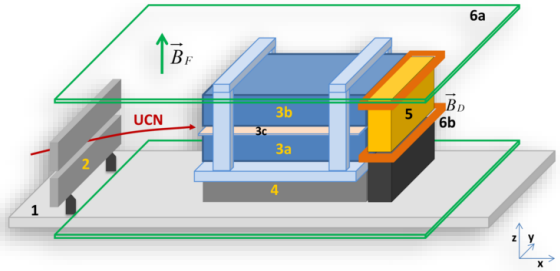


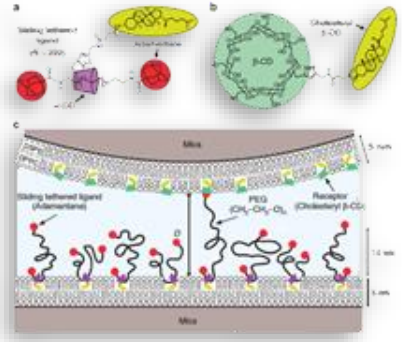


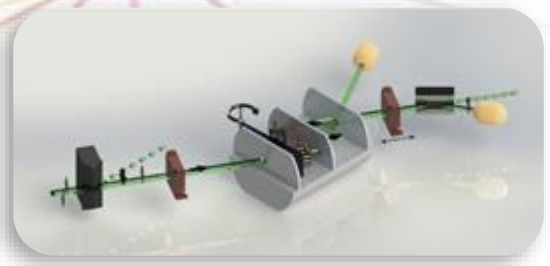


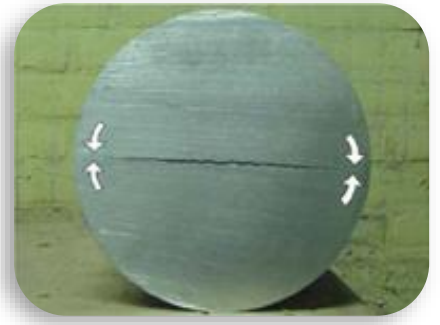


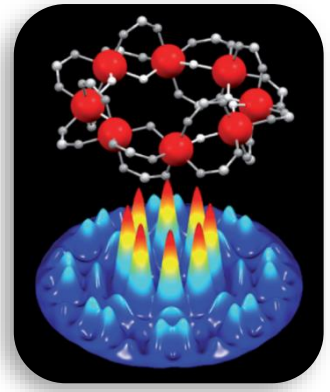












Electrically neutral: neutrons can penetrate deeply into matter

Yet they do not damage the studied sample

An engine in action

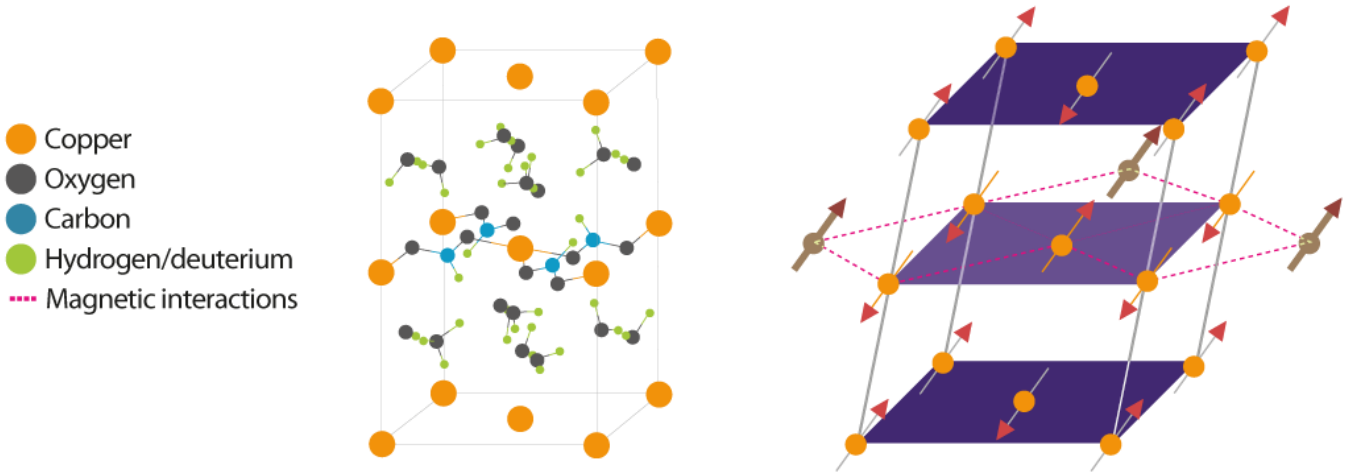
Jeremy H. Lakey J. R. Soc. Interface 2009;6:S567-S573

Plastic components are well resolved by neutrons owing to their hydrogen content while the metallic body is penetrated easily

Neutrons have a spin, therefore a sensitivity to magnetic properties

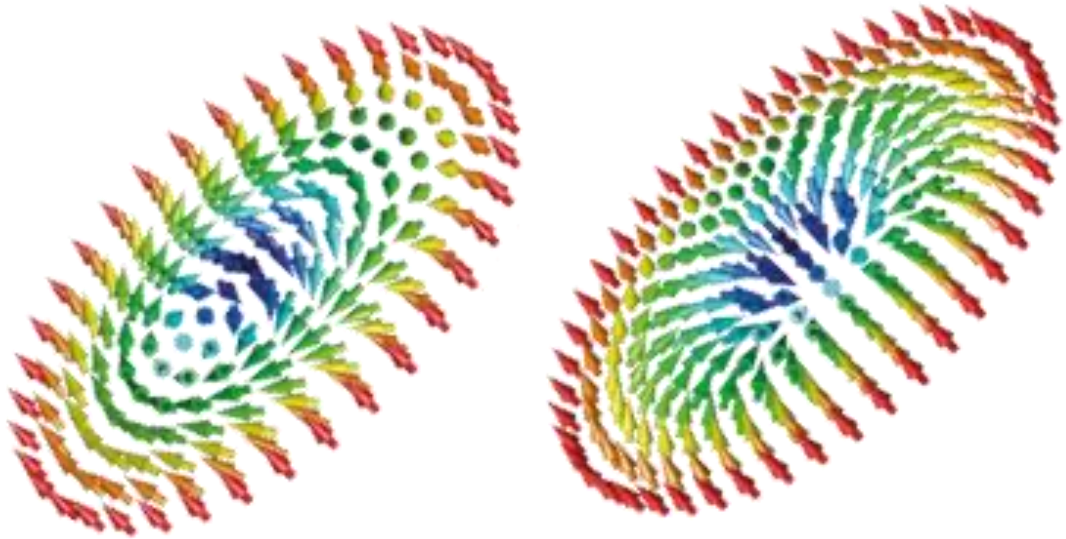
Beams of polarized neutrons (in which all the spins are aligned)

allow the characterization of exotic materials with complex structure and behavior



Copper formate:
crystal structure vs magnetic structure

Arrangement of spins in two different types of skyrmions

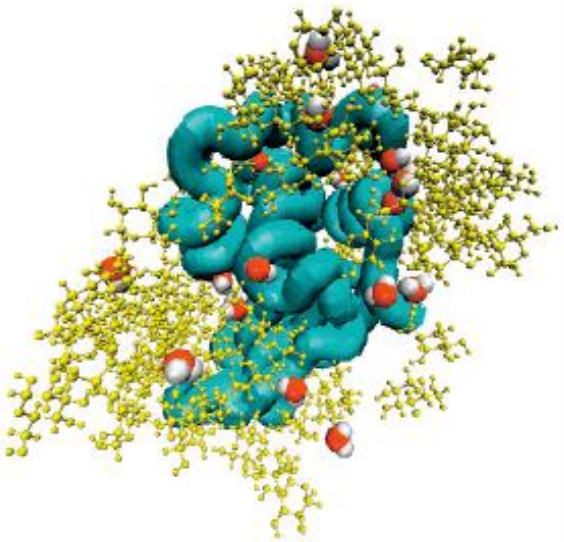


I. Kezsmarki et al., Nature Materials, 2015, **14**, 1116; DOI: 10.1038/nmat4402ptions.

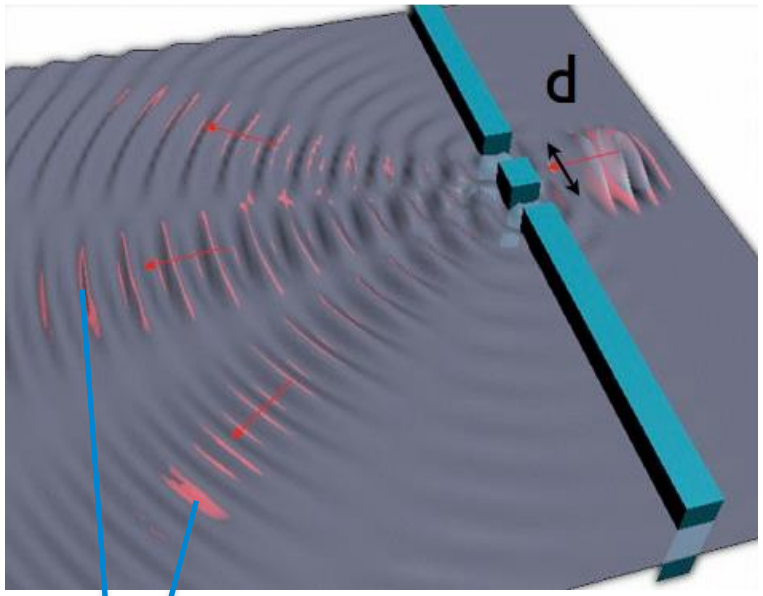
Neutrons wavelengths is comparable to atomic sizes

Adapted to the dimensions of atomic and molecular structures,
neutrons can « see » atoms, even in complex configurations.

From 1000 nm

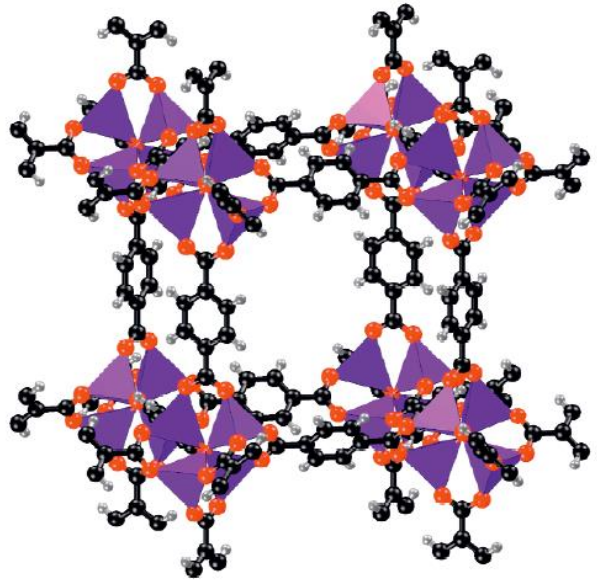


Cold neutrons



$$\Delta\phi = \frac{\Delta y}{D} = \frac{\lambda}{d}$$

To 0.001 nm

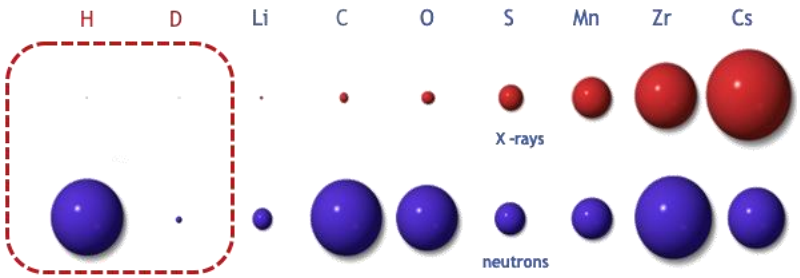


Hot neutrons

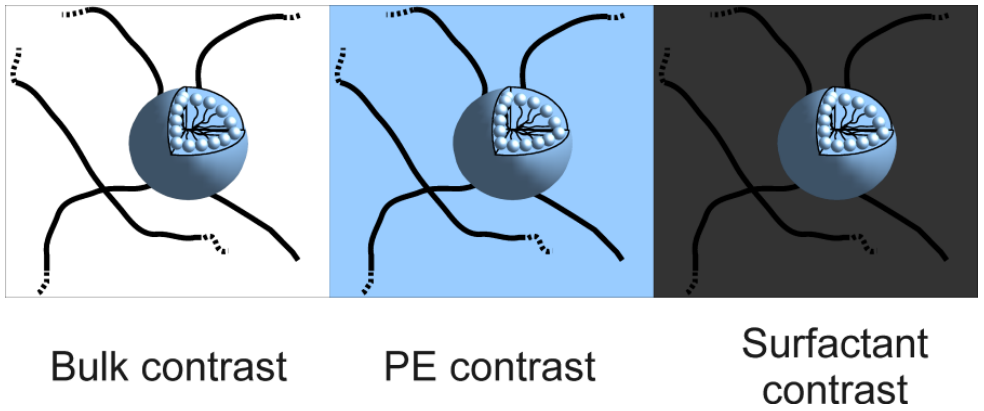
Why use neutrons to study soft an biological material?

Neutrons interact with nuclei

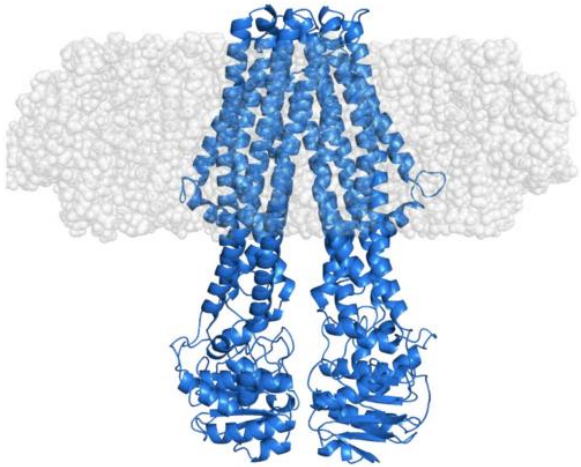
- are sensitive to light atoms, particularly hydrogen
- can exploit isotopic substitution, especially H/D
- ‘see‘ materials differently to X-rays, complementary



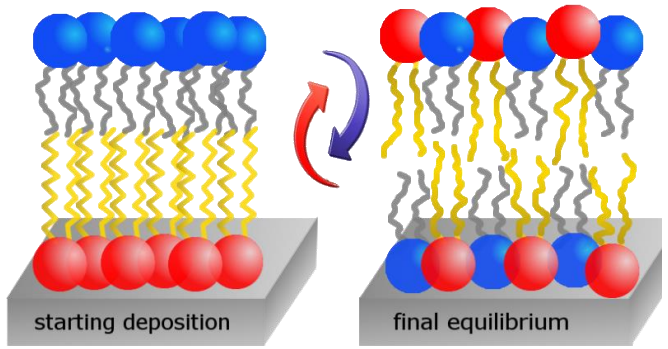
Polyelectrolyte + surfactant complex



Hoffmann et al. J Chem. Phys. 2015.



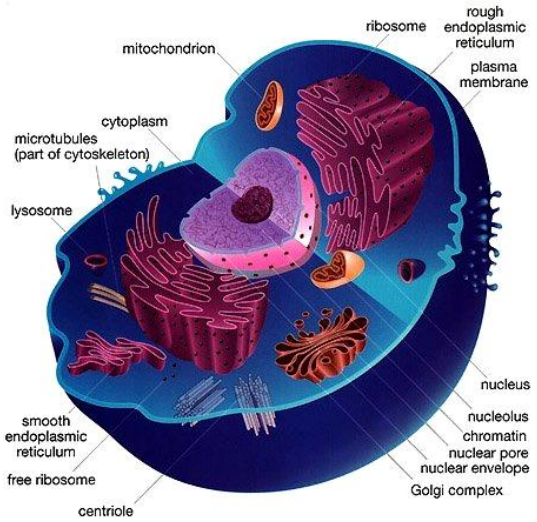
Josts et al. Structure 2018



Gerelli Y., et al., Langmuir 2012

NEUTRONS FOR SOCIETY

At the ILL the **structure of bio and soft matter** is probed by LSS instruments (small-angle scattering machines, reflectometers, small-angle diffractometers) while their **dynamics** is studied by neutron spectroscopy with motions probed from the fs time scale (eV) to ~100ns (neV), using inelastic scattering, backscattering, and spin-echo instruments.



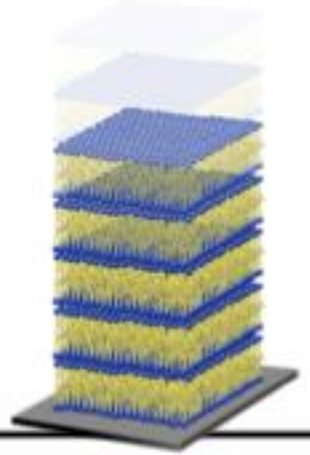
Energy storage

Structural

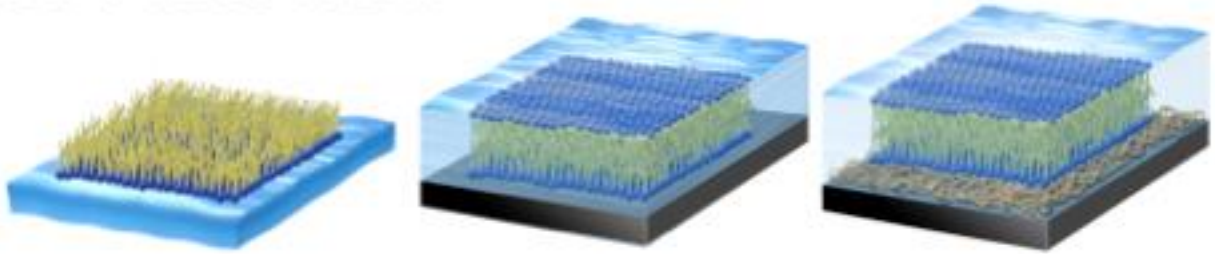
Signaling

PARTNERSHIP FOR SOFT CONDENSED MATTER

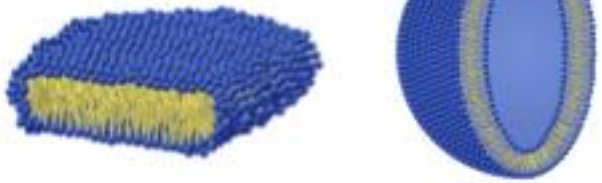
Model membranes and scattering techniques



DIFFRACTION



REFLECTIVITY



SANS

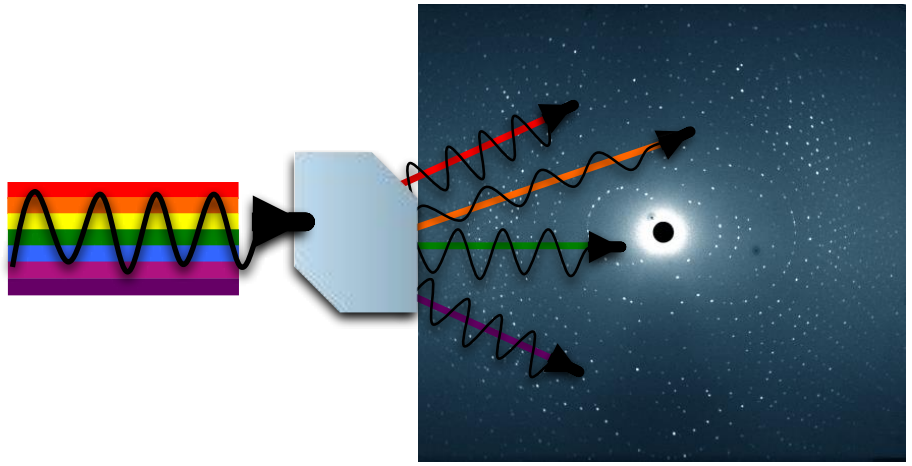
1 10 100 1000

Thickness Å

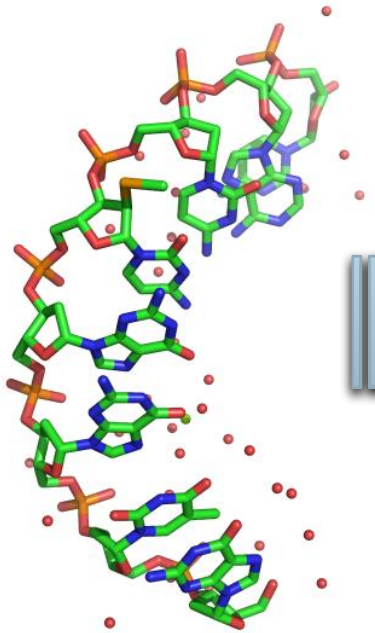
Neutron scattering techniques are ideally suited for the study of lipid bilayers (5nm thick) that are major components of cellular membranes. At the ILL, we have been working for several years to provide our users with well-characterized membrane models for physical and biological studies.

Neutron structure determination with LADI-III

1. **Reflection intensities** from neutron diffraction data are wavelength-normalized, scaled, merged and converted to structure factor amplitudes (F_{obs}).

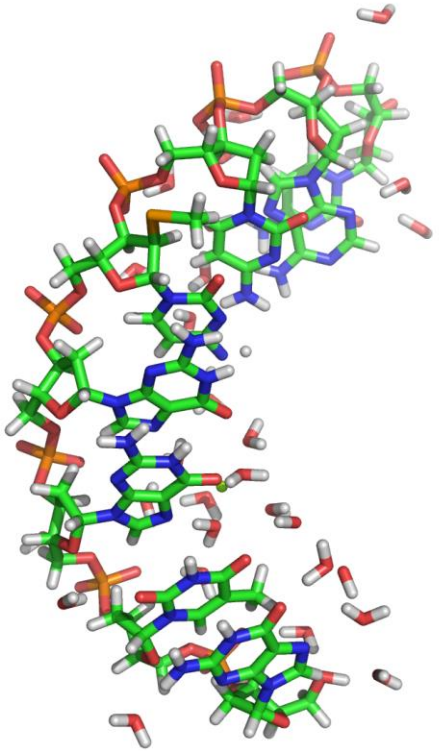


2. **Phase** information from an existing model determined using X-rays (*i.e.* C, N, O, S..).



Structural Refinement

'Neutron' structure includes the positions of ALL atoms!



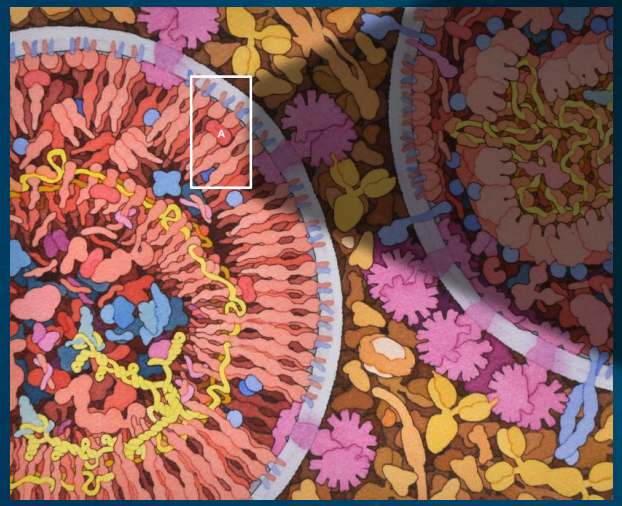
Neutrons reveal details of protonation, H-bonding and hydration which are essential for determining catalytic pathways and for understanding drug-binding

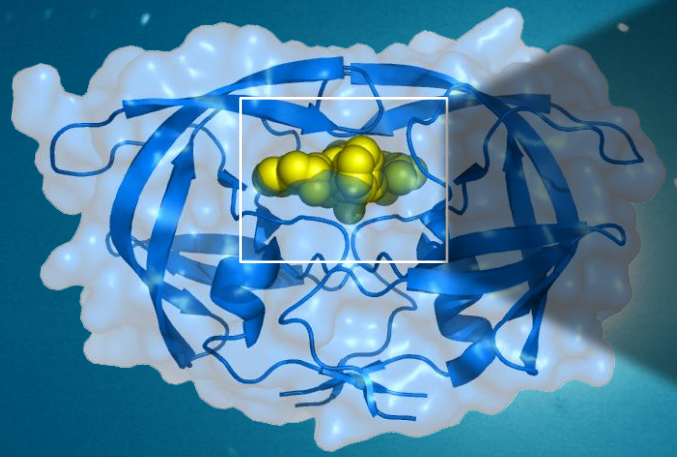
HIV-1 Protease drug-binding studies

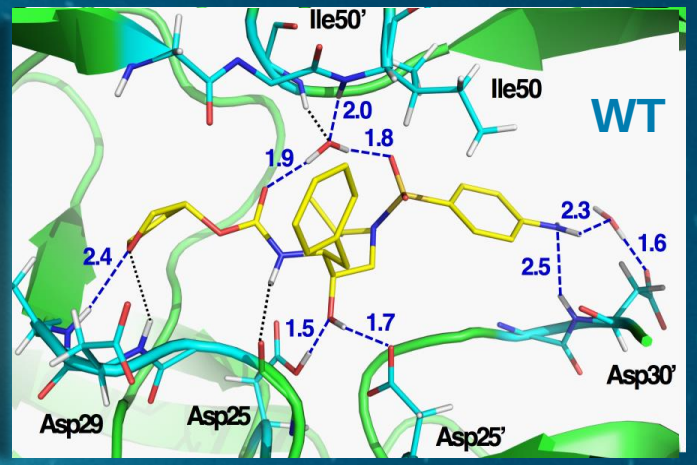
- **HIV-1 protease** is an essential enzyme in the **life-cycle of HIV** and is a clinical drug target
- Neutron studies have revealed how different clinical inhibitors bind, allowing us to suggest ways to **enhance the binding** and **limit drug-resistance**.

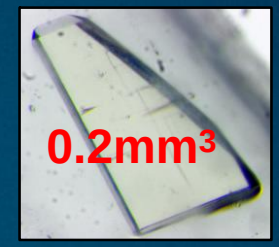
Andrey Kovalevsky (ORNL, USA)

RT studies of wild-type enzyme drug complexes, triple mutant enzyme drug complexes, and at different pHs









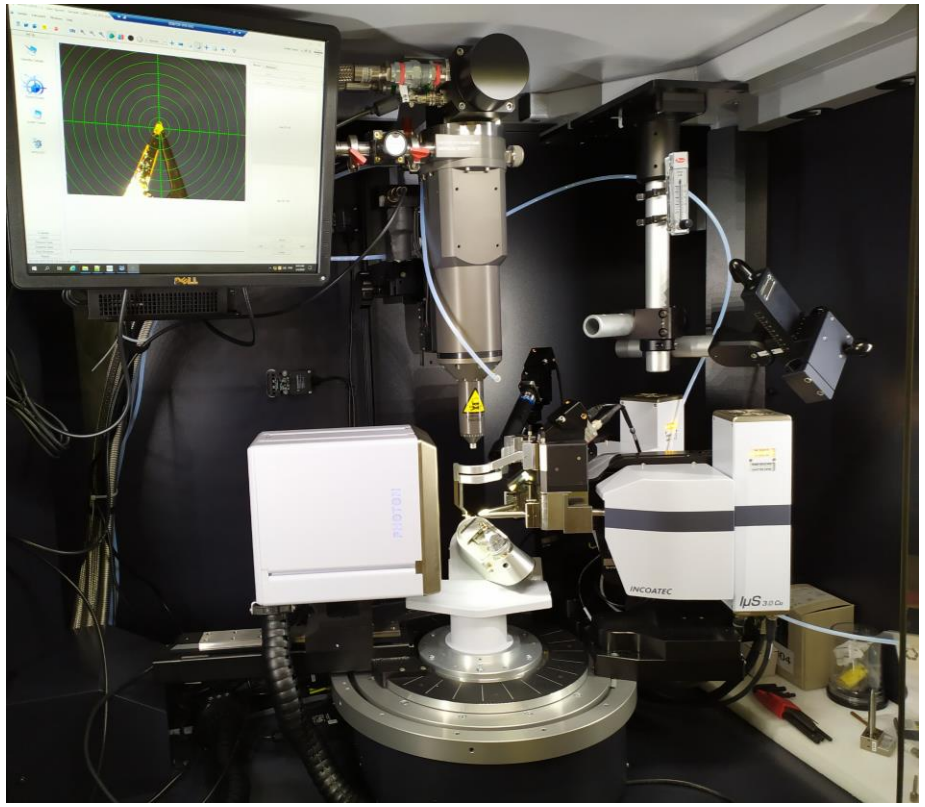
J. Med. Chem. (2013) 56, 5631

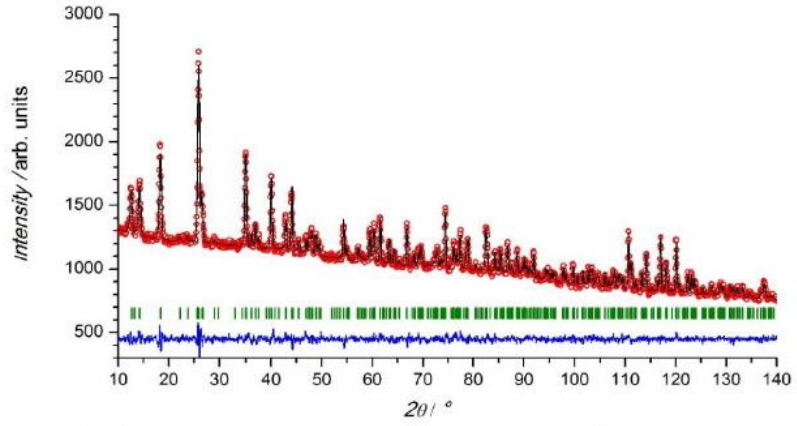
Angewandte Chem. (2016) 55, 4924

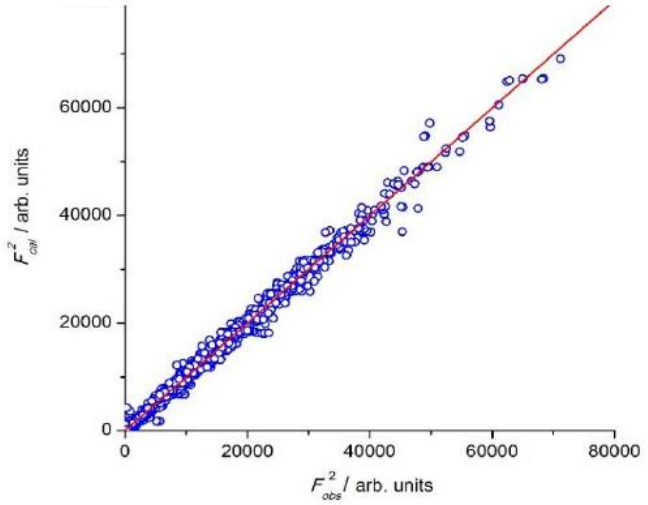
J. Med. Chem. (2017) 60, 2018

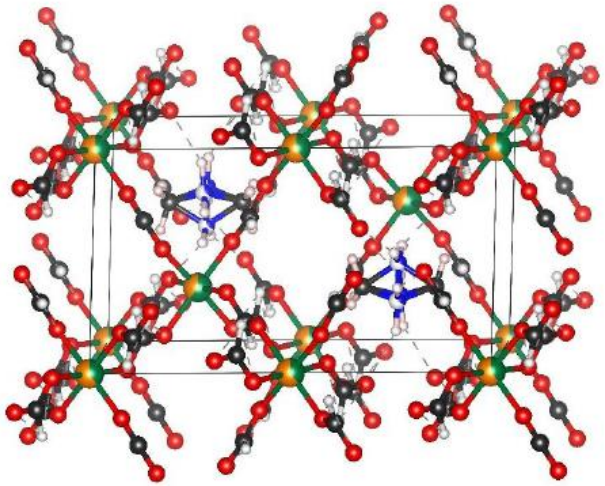
Single crystal diffraction – with X-rays!

Measuring N & X data – same sample & conditions



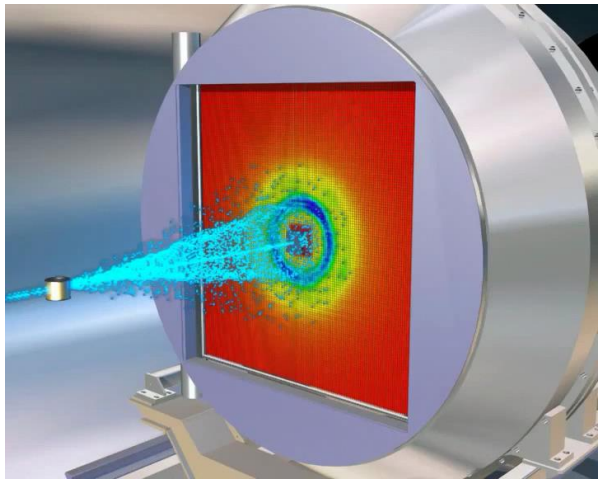






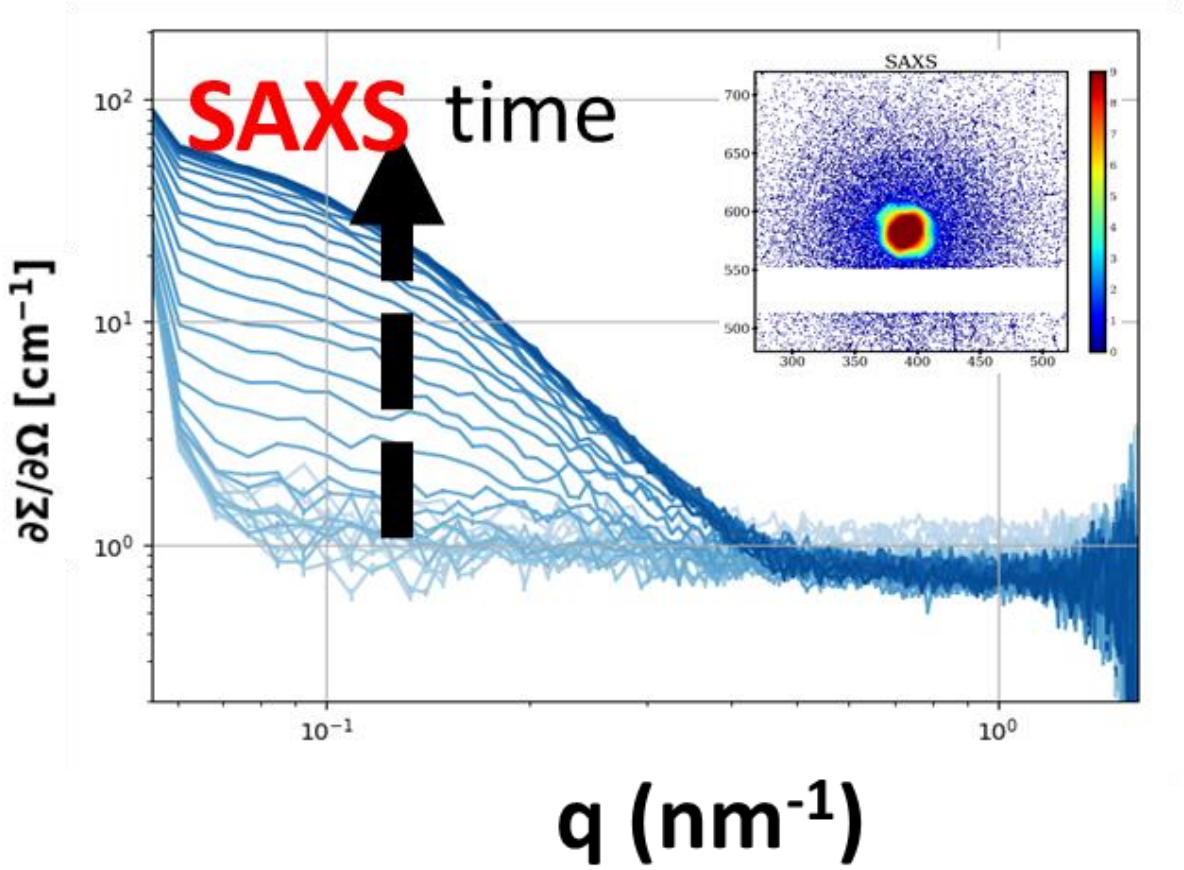
The access to the DRX instrument is already possible through Easy Access proposals via User Club.

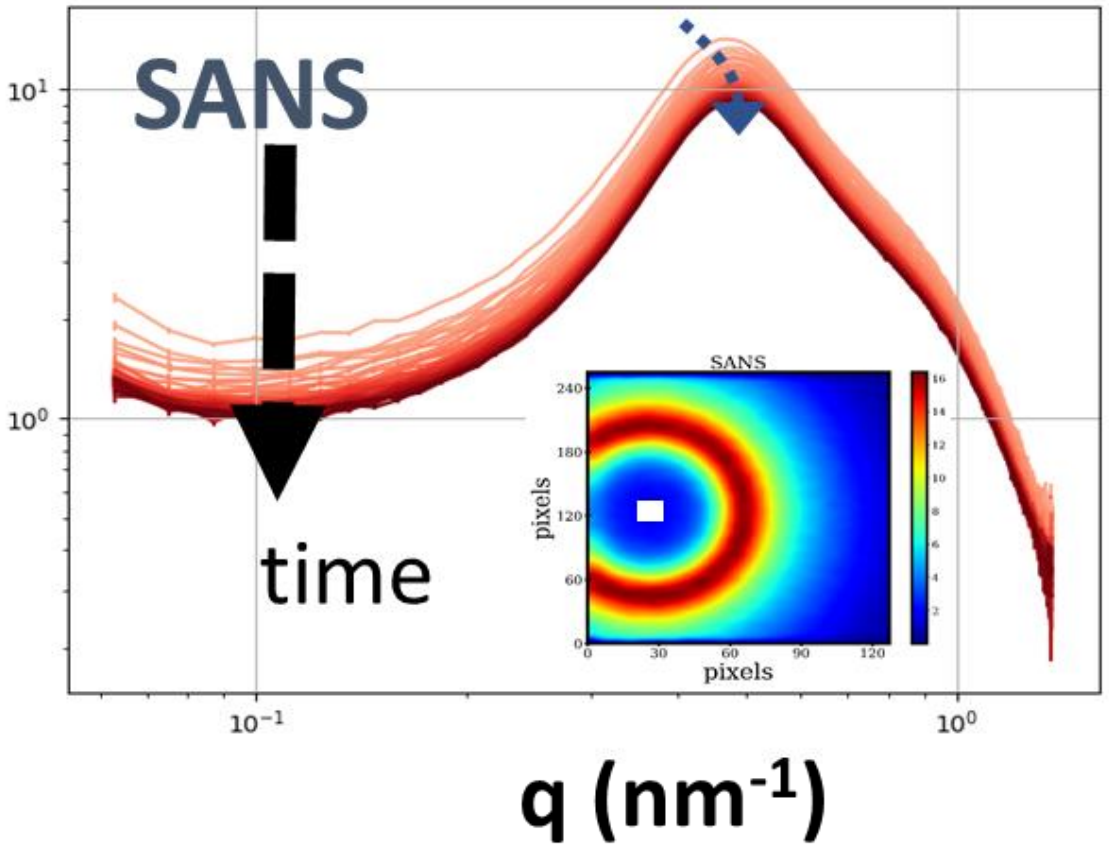
In-situ SAXS on D22



In-situ SAXS/SANS

Watching gold nanoparticles grow: Journal of Applied Crystallography **2020,** 53 (3).



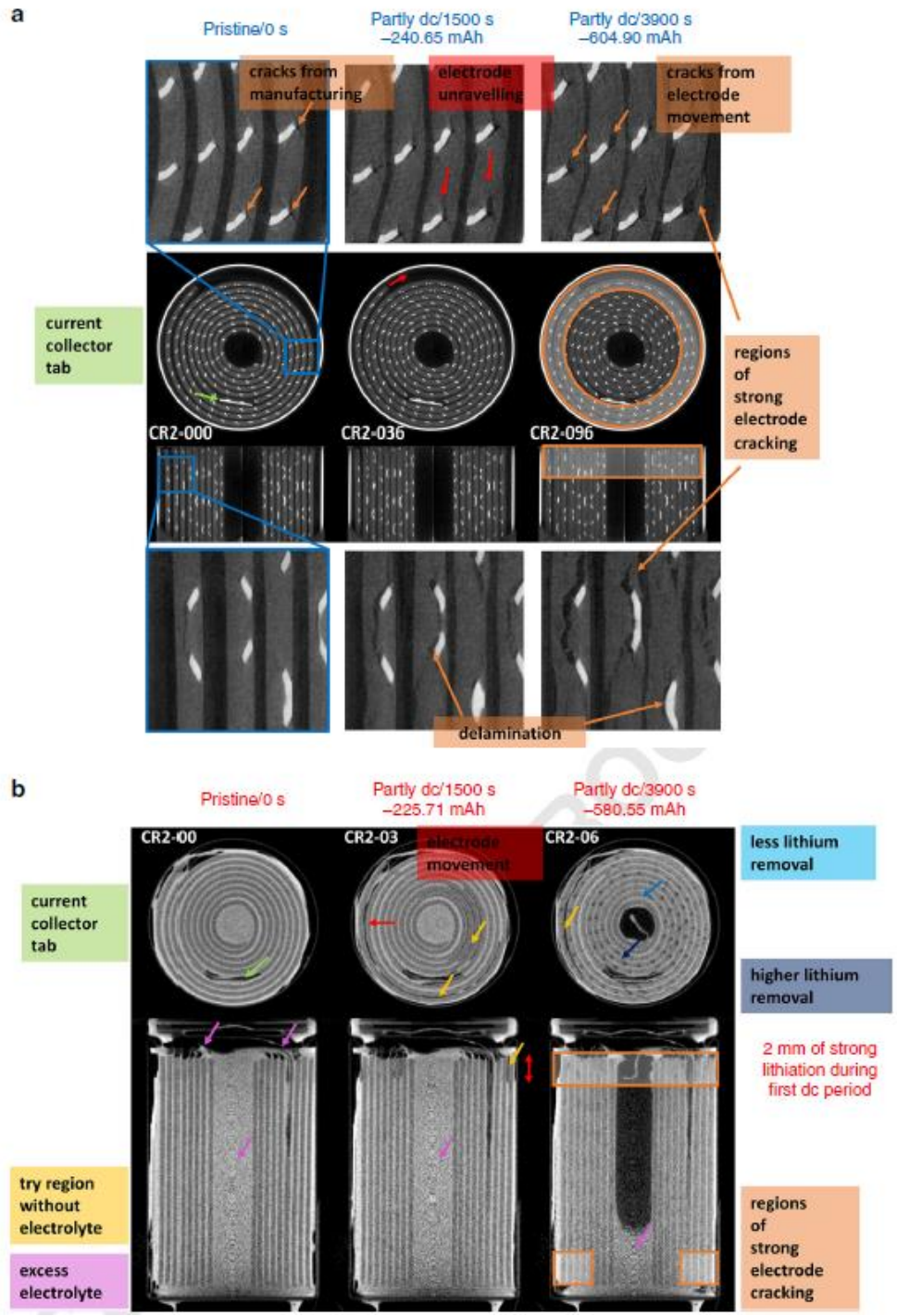


Imaging: D50 → NEXT

Public instrument: Partnership with UGA + HZB

Achievements on D50:

- ~3 *micron* resolution
- 1 *ms* images
- 1 *s* tomography
- simultaneous N+X with ~10 micron resolution (~85% of experiments)



Nature Communications
https://doi.org/10.1038/s41467-019-13943-3

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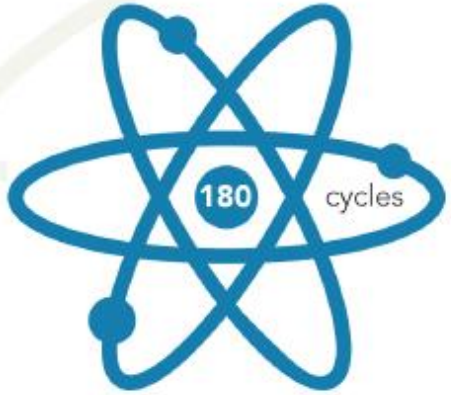

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