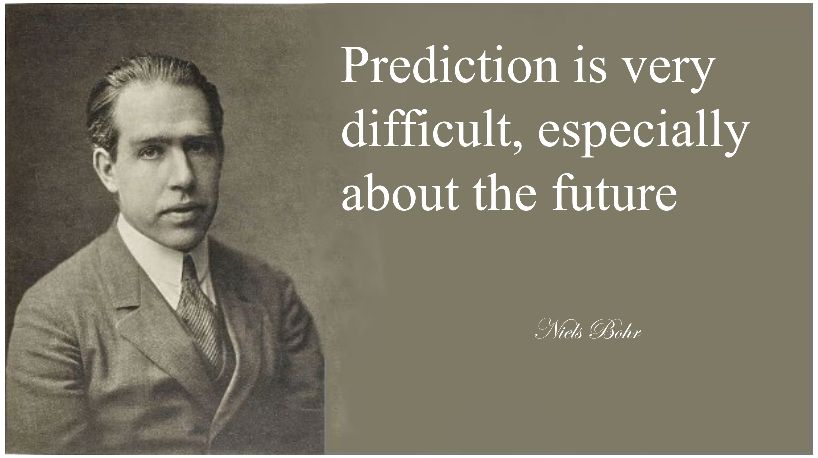
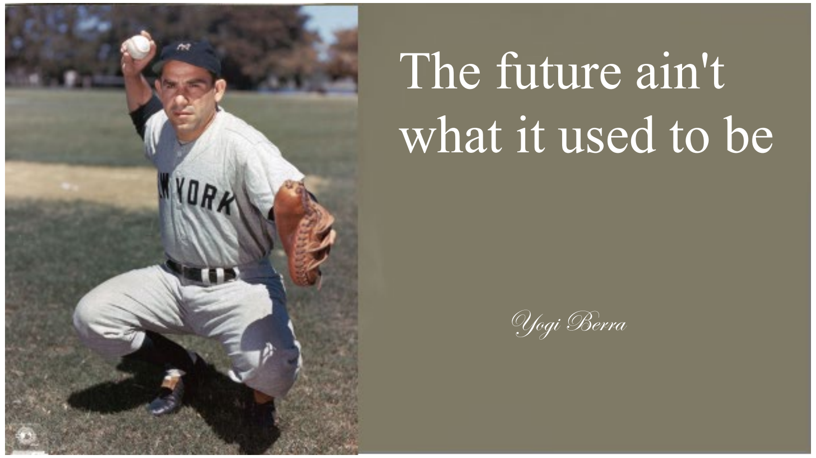
Oxford Physics

UNIVERSITY OF OXFORD

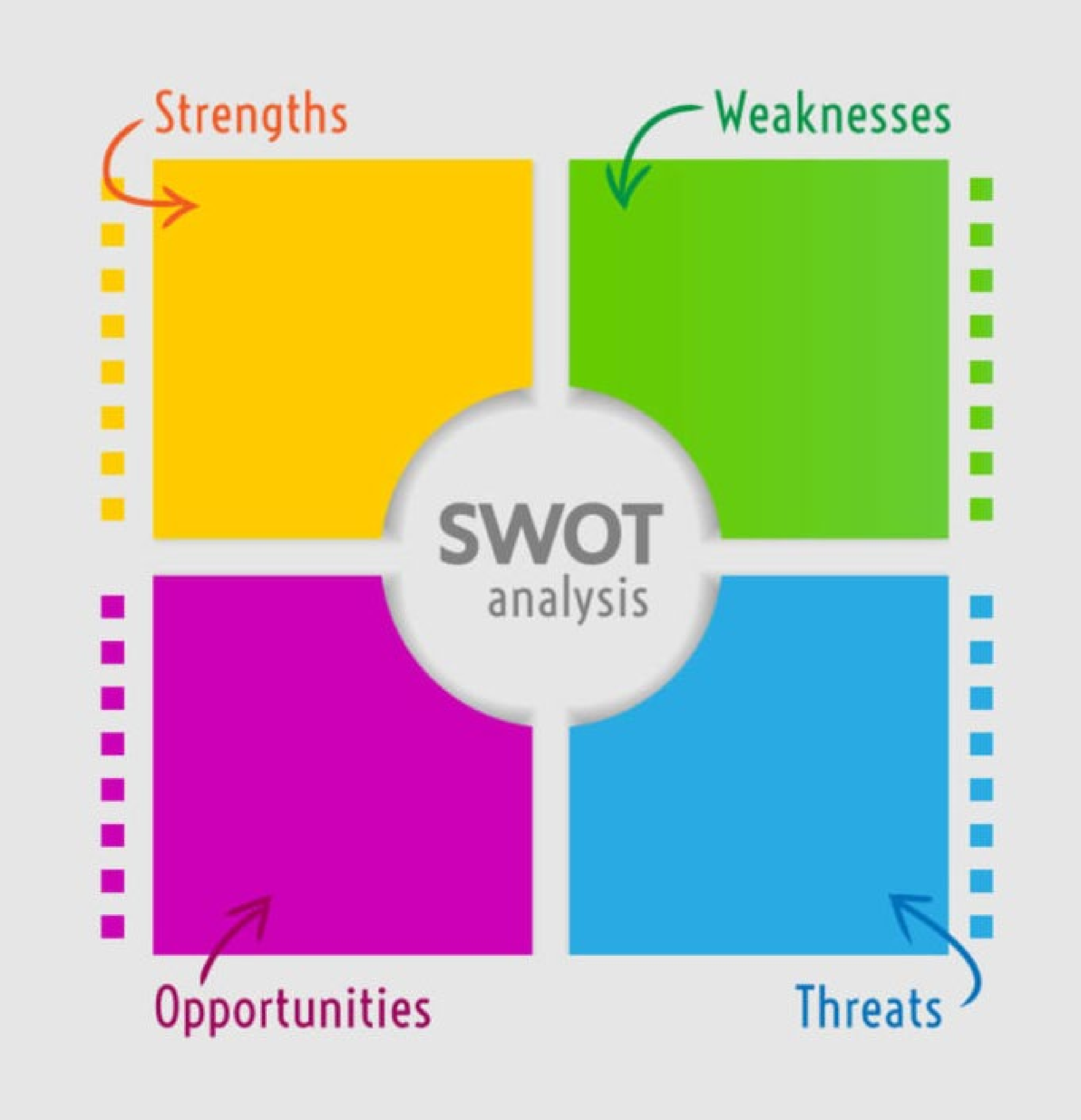




The future of neutrons

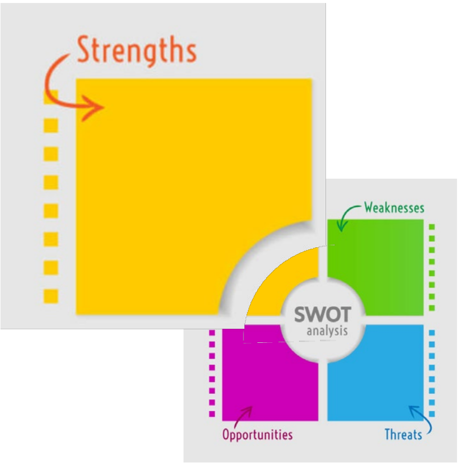
Paolo G. Radaelli
Clarendon Laboratory, University of Oxford

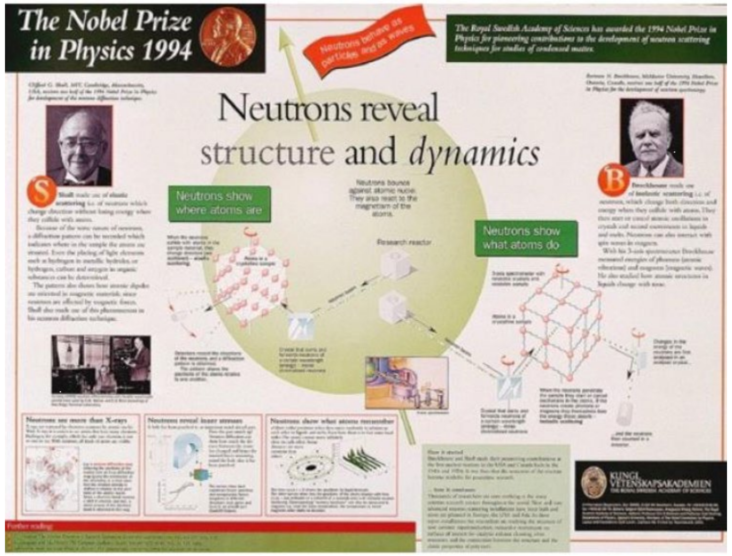
50 years of UK@ILL: Grenoble, 29 November 2023

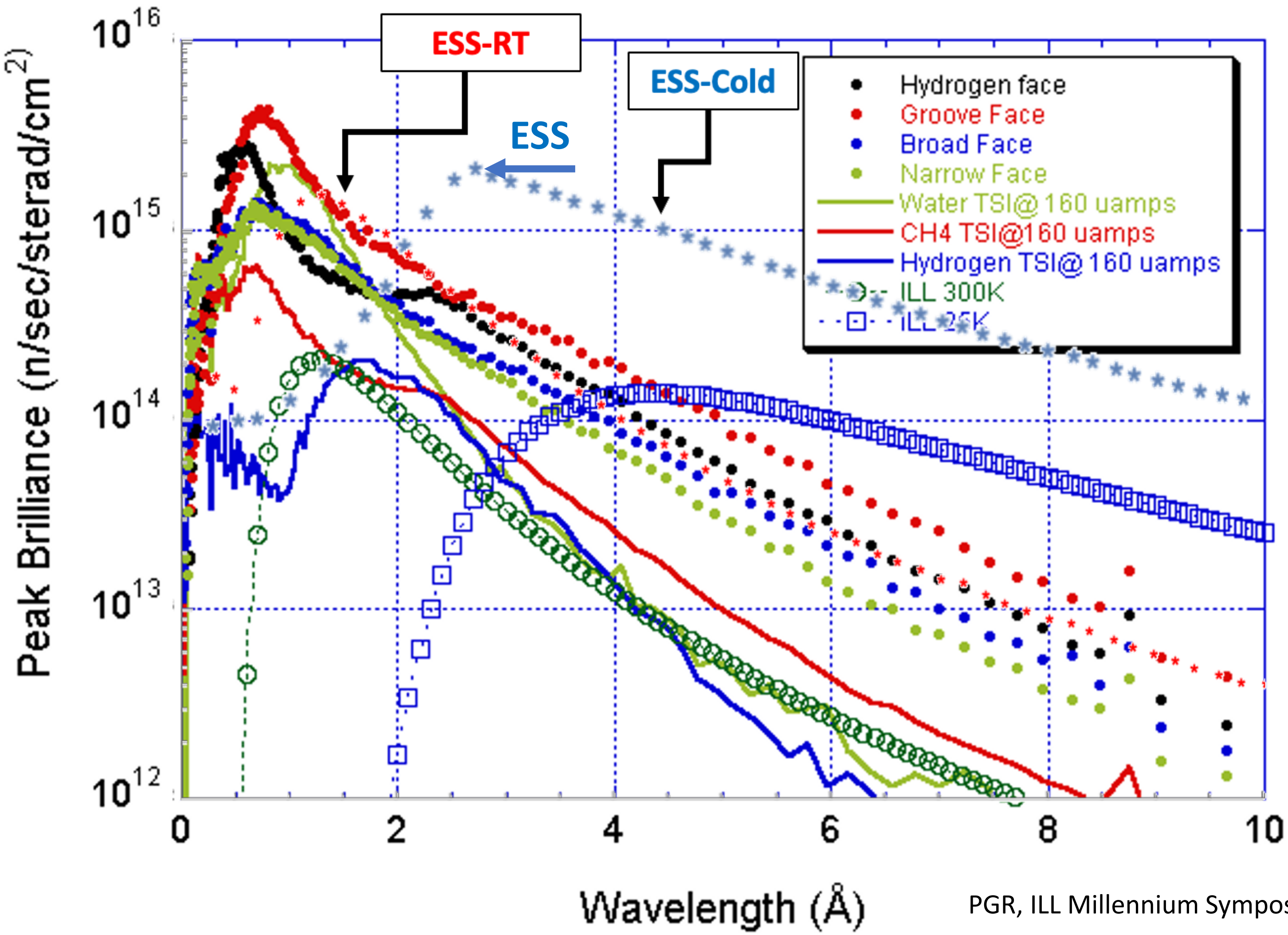

Strengths
Weaknesses
SWOT
analysis
Opportunities
Threats

Neutrons are great!

and I mean <u>really</u> great

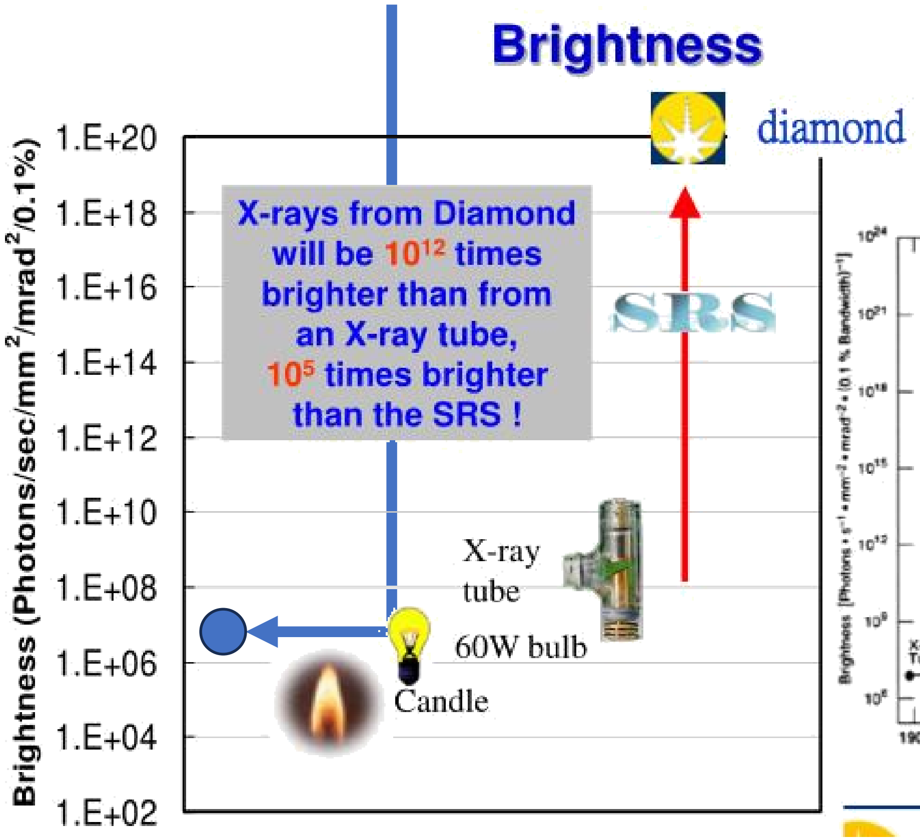




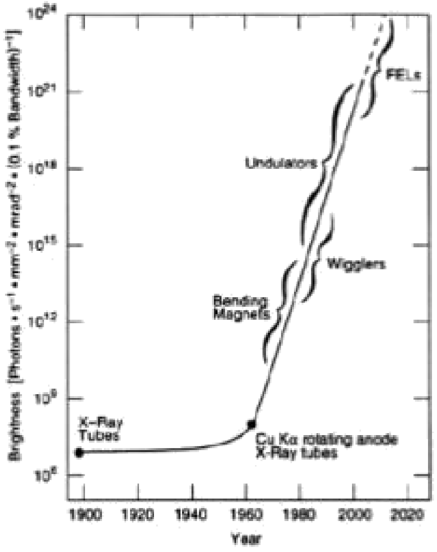


PGR, ILL Millennium Symposium, April 2006

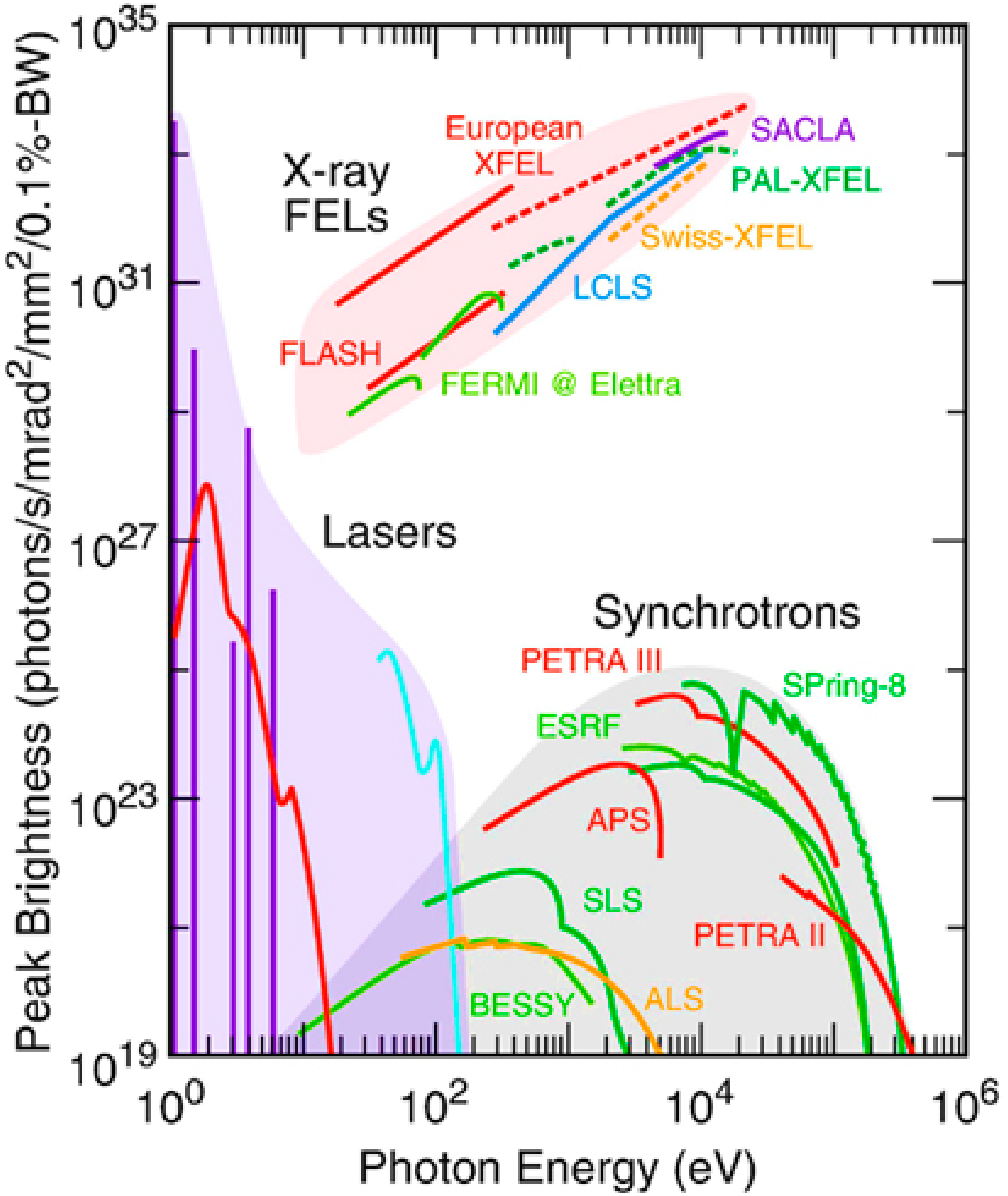
ESS@5MW



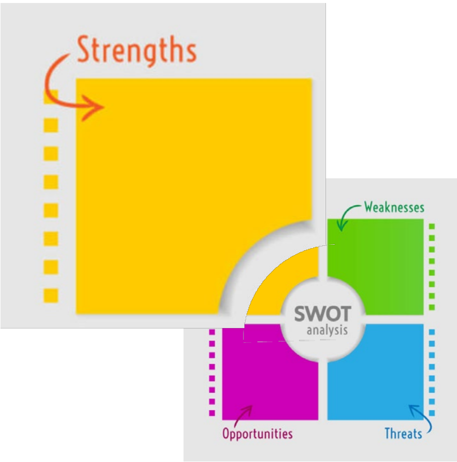
Brightness
diamond
X-rays from Diamond will be 10^12 times brighter than from an X-ray tube, 10^5 times brighter than the SRS !
SRS
X-ray tube
60W bulb
Candle
Brightness (Photons/sec/mm^2/mrad^2/0.1%)
1.E+20
1.E+18
1.E+16
1.E+14
1.E+12
1.E+10
1.E+08
1.E+06
1.E+04
1.E+02



FELs
Undulators
Wigglers
Bending Magnets
X-Ray Tubes
Cu Kα rotating anode X-Ray tubes
1900
1920
1940
1960
1980
2000
2020
Year



X-ray FELs
European XFEL
SACLA
PAL-XFEL
Swiss-XFEL
LCLS
FLASH
FERMI @ Elettra
Lasers
Synchrotrons
PETRA III
SPring-8
ESRF
APS
SLS
PETRA II
BESSY
ALS
Peak Brightness (photons/s/mrad^2/mm^2/0.1%-BW)
10^35
10^31
10^27
10^23
10^19
10^0
10^2
10^4
10^6
Photon Energy (eV)



There are/will be rather a lot of them available

…at least now, specially for UK scientists

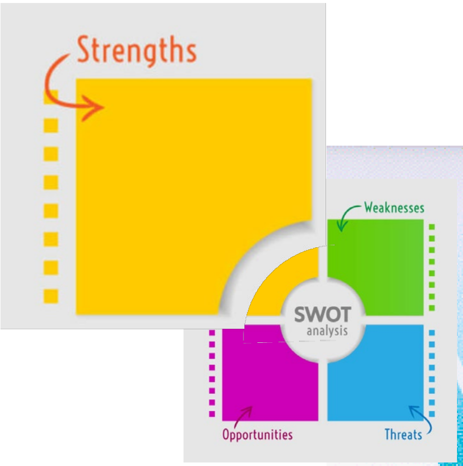
NEUTRONS FOR SOCIETY

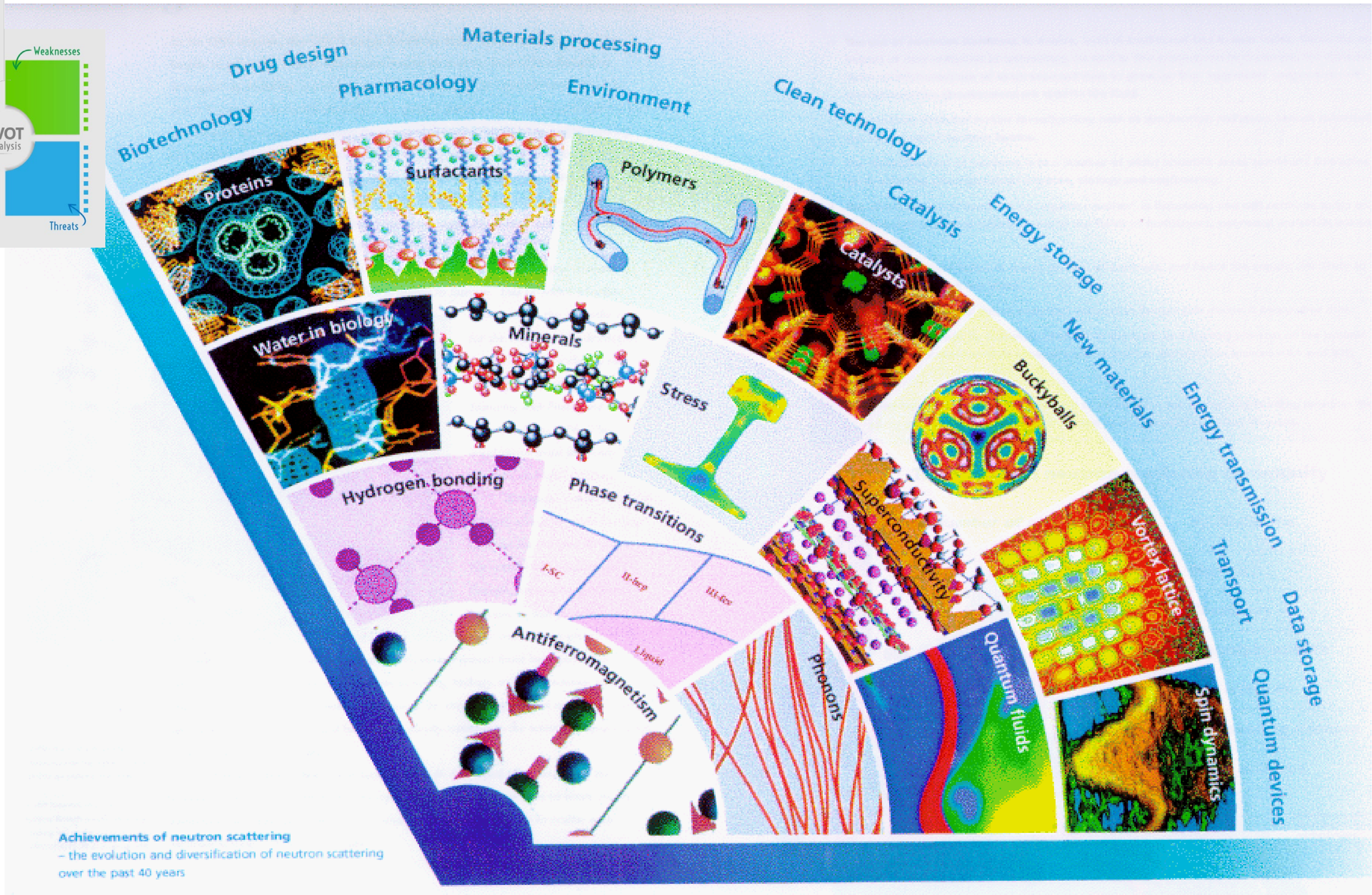
Science and Technology Facilities Council

ISIS Neutron and Muon Source

EUROPEAN SPALLATION SOURCE

A wide spectrum of science and technology

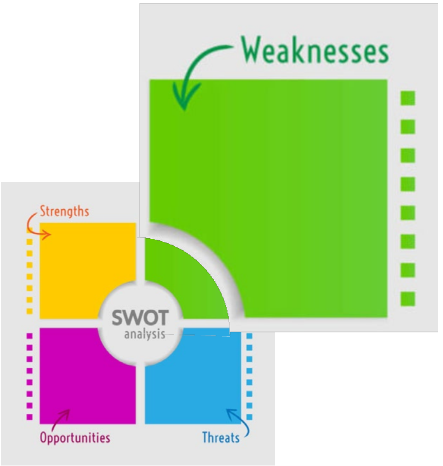




Source: A.D. Taylor

*Not many weakness**es but some….***

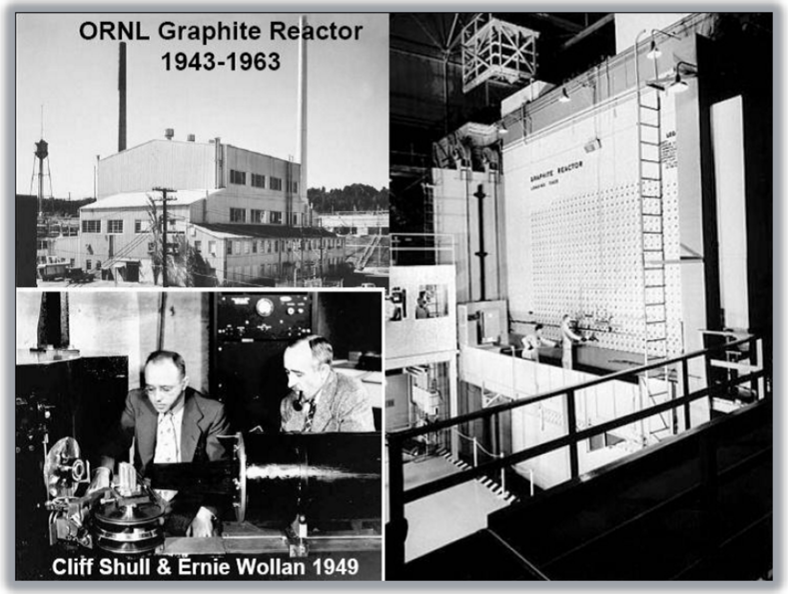
specifically for the UK

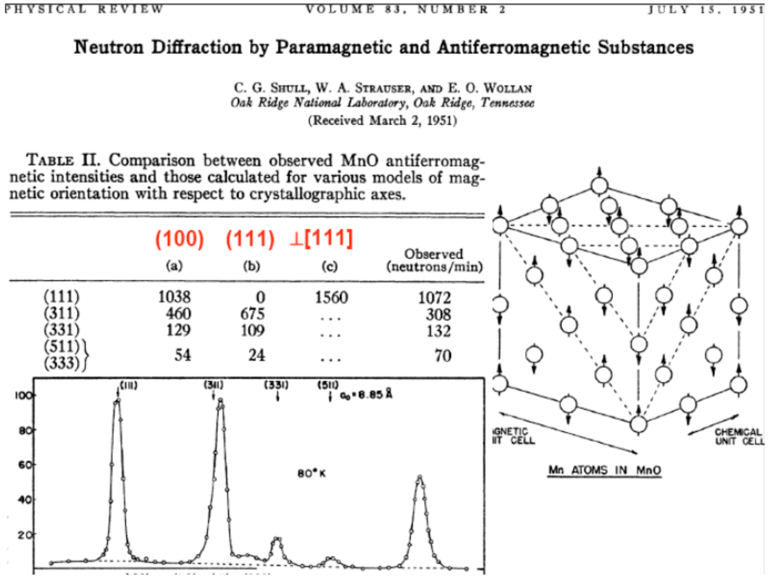


- Little **direct community involvement** with sources/instrumentation, e.g., compared with our colleague in PP or Astro. The disengagement with ESS is a particularly egregious case…
- The UK neutron community needs to fight '**one grant at a time**', often against UKRI priority areas that seem somewhat disconnected with the worldwide landscape (again, compare/contrast with PP/Astro consolidated grants).
- #1 challenge – **Quantum Materials** (SNS-STS) not in strong focus in UK.
- The **'high-impact' science** base may be narrower than one thinks…

First determination of magnetic structure performed at ORNL

- Clifford G. Shull received 1994 Nobel prize in Physics.





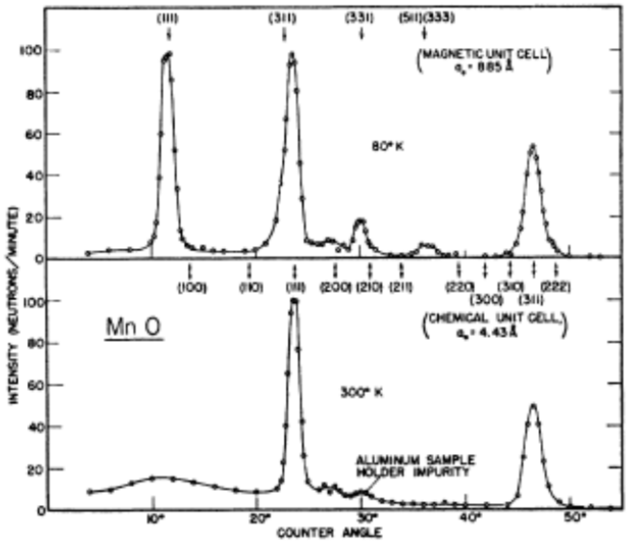
PHYSICAL REVIEW VOLUME 83, NUMBER 2 JULY 15, 1951

Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances

C. G. Shull, W. A. Strauser, and E. O. Wollan
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received March 2, 1951)

Table II. Comparison between observed MnO antiferromagnetic intensities and those calculated for various models of magnetic orientation with respect to crystallographic axes.

	(100) (a)	(111) (b)	⊥[111] (c)	Observed (neutrons/min)
(111)	1038	0	1560	1072
(311)	460	675	...	308
(331)	129	109	...	132
(511) (333)	54	24	...	70



- First direct evidence of antiferromagnetism in MnO.
- Neel model of ferrimagnetism confirmed in Fe_3O_4.
- First magnetic form-factor data obtained in Mn compounds.
- Production of polarized neutrons by Bragg reflection from ferromagnets demonstrated.

Credit: Stuart Calder, ORNL

piest ordered perovskite structures with a $YBa_2Cu_3O_y$ stoichiometry consists of 1:1:*n* stacking of cubic perovskite building blocks with Cu atoms on the cube corners, Y or Ba atoms in the center of the cube, and O atoms on the cube edges. From powder x-ray diffraction data Cava *et al.*[3] proposed an orthorhombic unit cell with $a \approx 3.822$ Å, $b \approx 3.891$ Å, $c = \approx 11.677$ Å. Grant *et al.*[4] proposed a tetragonal unit cell with $a \approx 3.89$ Å and $c \approx 11.65$ Å. Both reports speculate that the structure of the superconducting material is a 1:1:3 variant of the perovskite unit cell with ordered Y and Ba cations and an unspecified number of oxygen atoms. A single-crystal x-ray diffraction study by Hazen *et al.*[6] determined the structure of $YBa_2Cu_3O_x$ (x reported as ≈ 6.5) as tetragonal with space group $P\bar{4}m2$ and confirmed the 1:1:3 stacked perovskite derivative structure. This structure contains CuO_2 planes and ordered oxygen vacancies in the BaO and YO planes. In all of these studies the oxygen atom p

this system. The sample studied here exhibits, previously reported,[2] a metallic resistance toge sharp superconducting transition at 92.5 K width of 3 K) which shows that the supercondu is homogeneous.

Neutron powder diffraction data were colle sample of $YBa_2Cu_3O_y$ using the special-enviro der diffractometer at the Intense Pulsed Neu (IPNS) and analyzed with the Rietveld struc ment technique.[7] The sample was found to hav orthorhombic 1:1:3 ABO_3 perovskite structure space group and lattice constants $a = 3.8$ $b = 3.8864(1)$ Å, and $c = 11.6807(2)$ Å simi proposed by Cava *et al.*[3] Three orthorhombic s were modeled: $Pmm2$, $P222$, and $Pmmm$. The st initially solved in the acentric space group Pm of Cu atoms at the positions (0

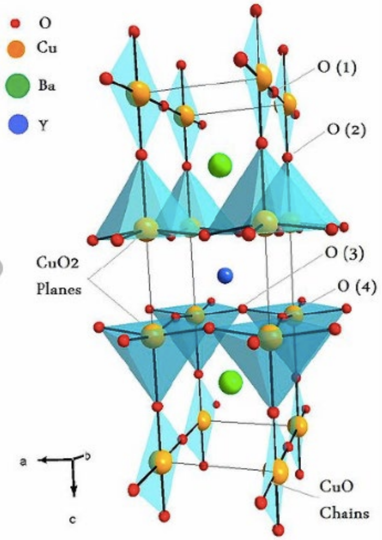
Jim Jorgensen

we have no means of determining whether defects play any direct role in the superconducting properties of these materials

We acknowledge valuable discussions with Janet Brown, J M. Cowley, W. J. Skocpol and S. Zahurak. The low-temperature experiments were partially supported by the NSF.

Note added in proof: We have recently learned of neutron diffraction experiments by J. J. Capponi *et al. Europhys. Lett* 3, 1301–1308 (1987) which also indicate the presence of long range order in the oxygen vacancies.

Received 16 April; accepted 6 May 1987.



RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 35, NUMBER 16 1 JUNE 1987

Oxygen ordering in the crystal structure of the 93-K superconductor $YBa_2Cu_3O_7$ using powder neutron diffraction at 298 and 79.5 K

J. E. Greedan and A. H. O'Reilly
Department of Chemistry, Institute for Materials Research, McMaster University, Hamilton, Canada L8S 4M1

C. V. Stager
Department of Physics, Institute for Materials Research, McMaster University, Hamilton Canada L8S 4M1

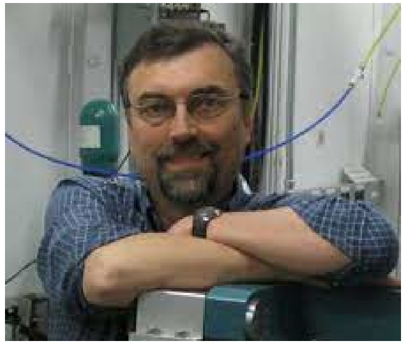
(Received 30 March 1987)

EUROPHYSICS LETTERS 15 June 1987

Europhys. Lett., 3 (12), pp. 1301-1307 (1987)

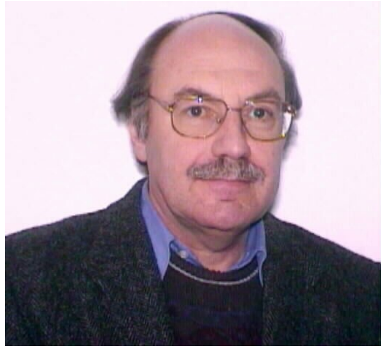
Structure of the 100 K Superconductor $Ba_2YCu_3O_7$ between (5 ÷ 300) K by Neutron Powder Diffraction.

J. J. Capponi (*), C. Chaillout (*), A. W. Hewat (**), P. Lejay (***), M. Marezio (*_*), N. Nguyen (_*_), B. Raveau (_*_), J. L. Soubeyroux (**), J. L. Tholence (***) and R. Tournier (***)



Carlo Segre

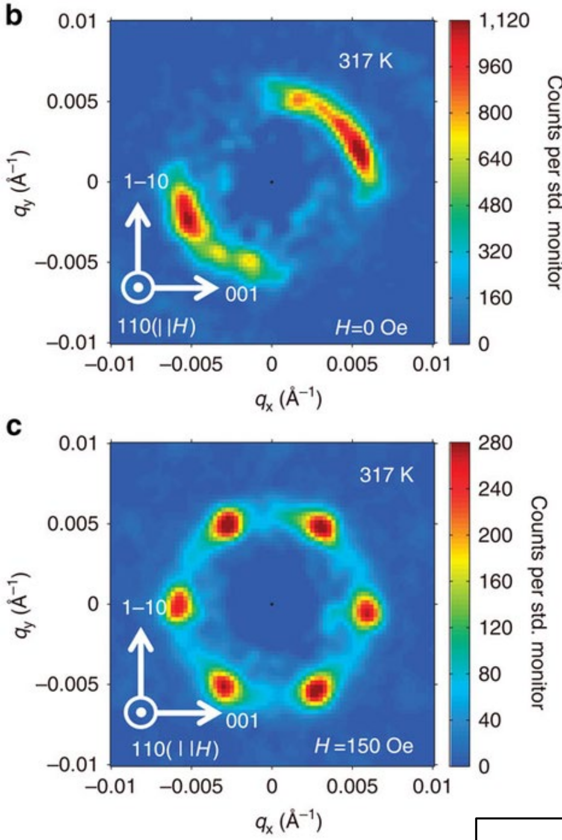
Bill David

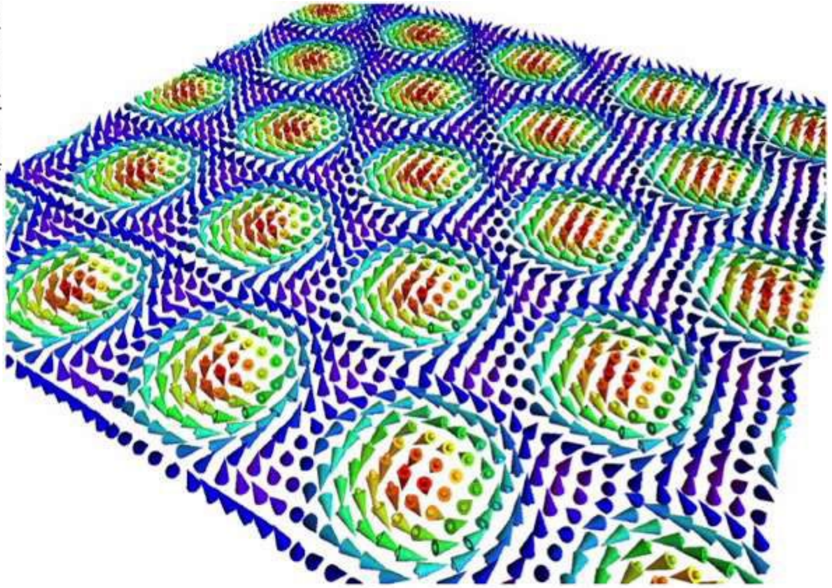


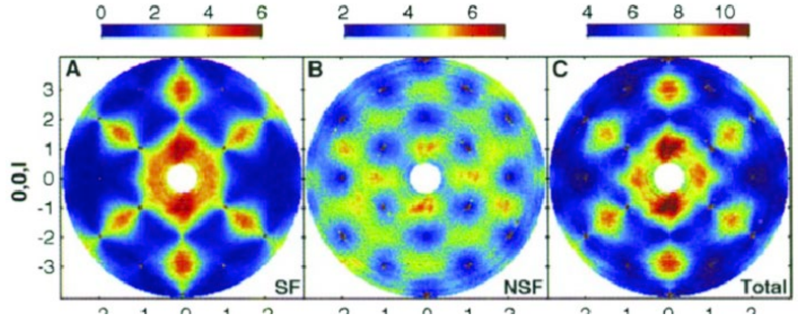
Alan Hewat

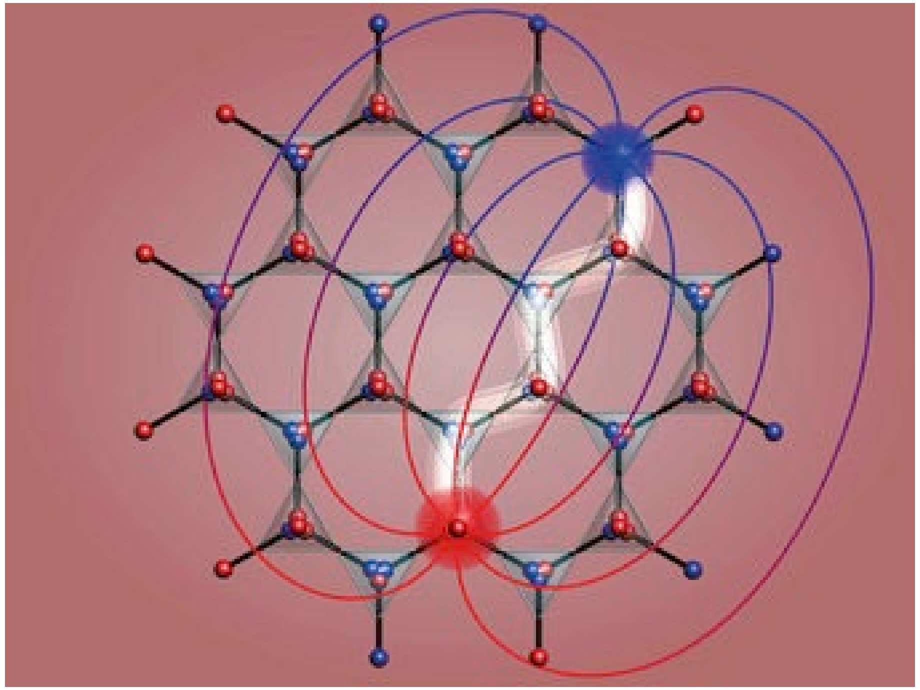
Massimo Marezio

…and more recently…





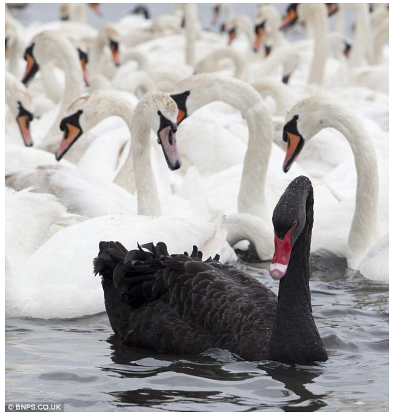


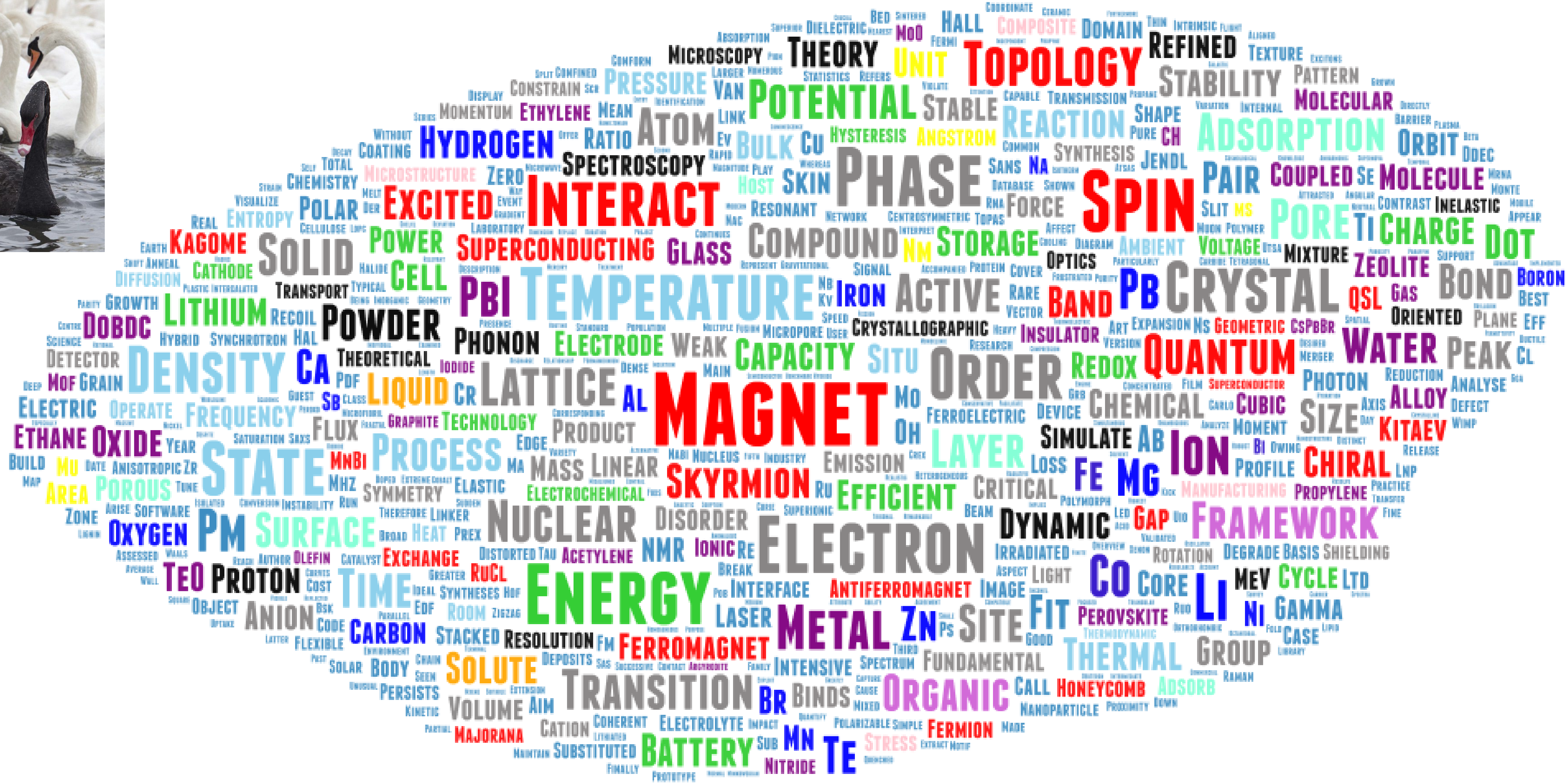


Spin ice/monopoles

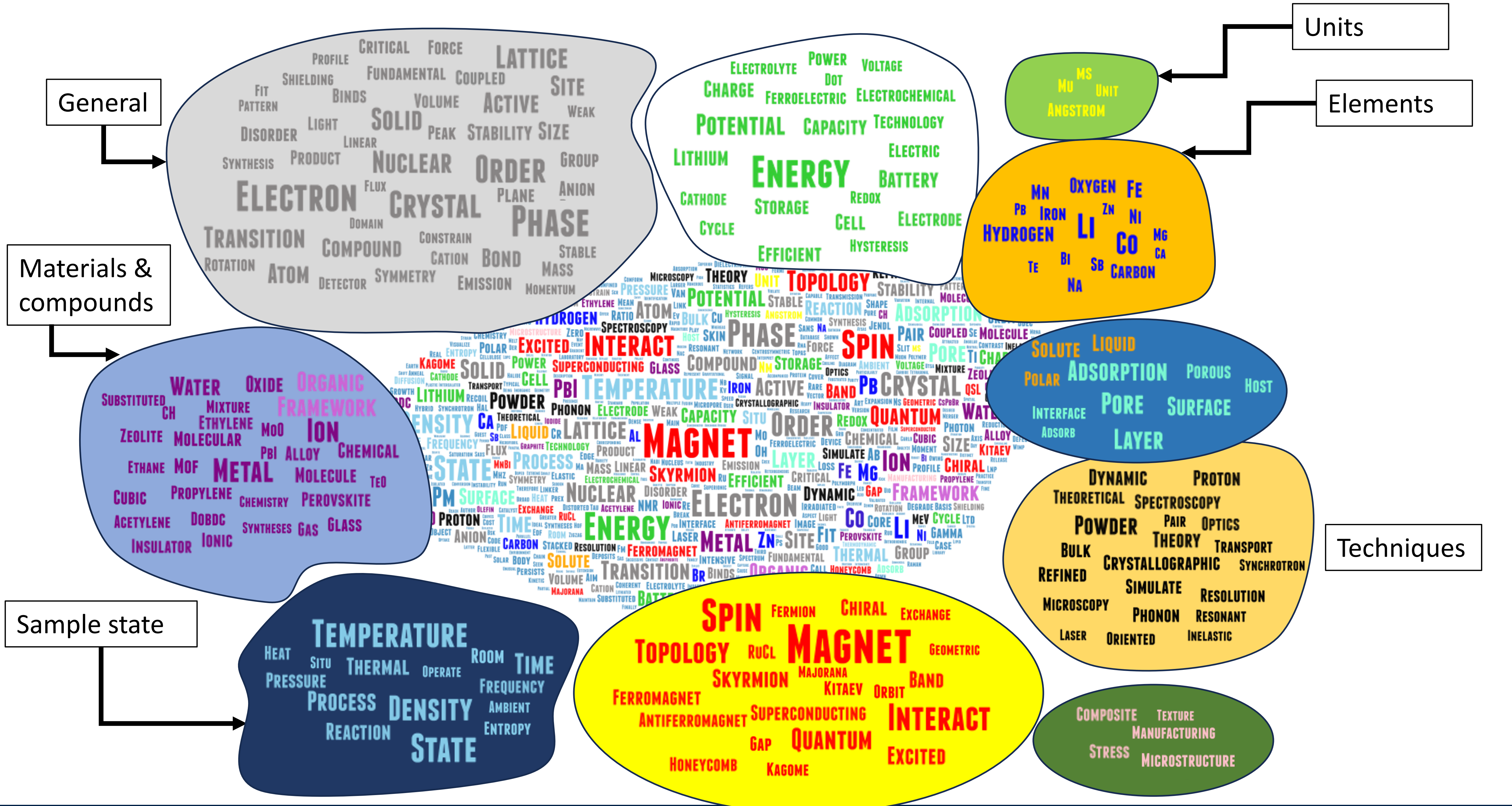
Magnetic skyrmions

185 Clarivate® Highly Cited Papers (top 1%) 2000-2024[†]

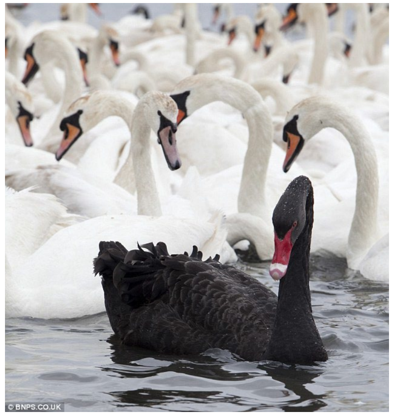




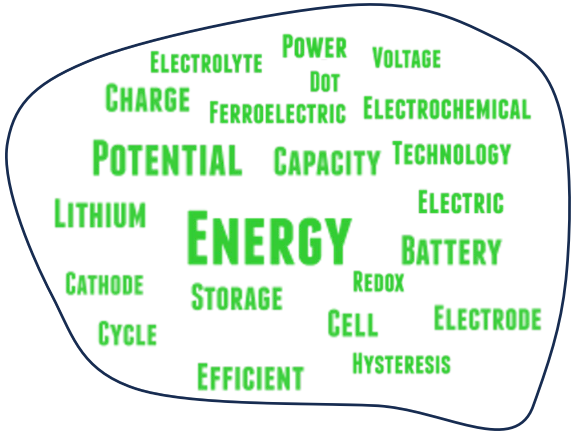
[†]Excluding 'neutron', 'structure' and common words

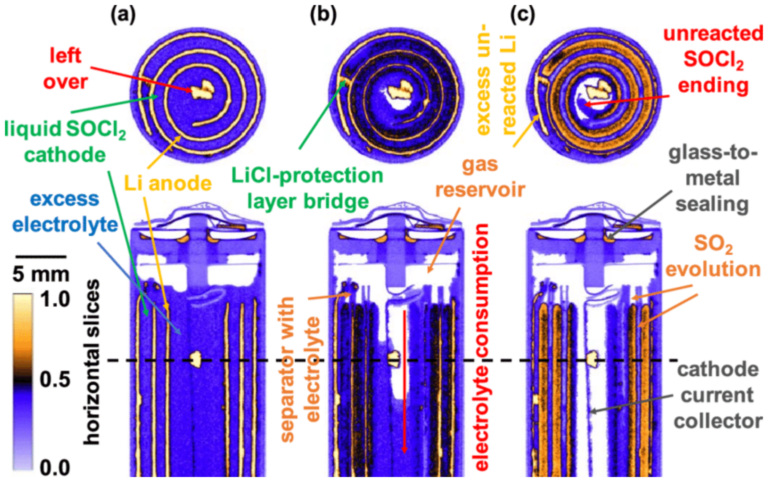


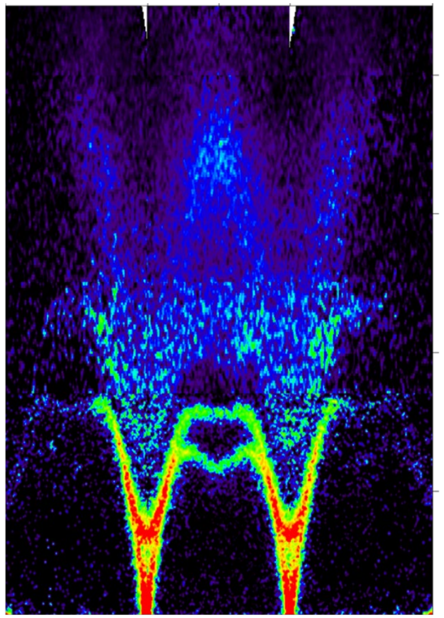
General
Critical Force Lattice Profile Fundamental Coupled Site Fit Shielding Binds Volume Active Weak Pattern Solid Disorder Light Peak Stability Size Linear Synthesis Product Nuclear Order Group Electron Flux Crystal Plane Anion Domain Phase Transition Compound Constrain Stable Rotation Atom Cation Bond Mass Detector Symmetry Emission Momentum
Materials & compounds
Water Oxide Organic Substituted Mixture Framework CH Ethylene MoO Ion Zeolite Molecular Chemical PbI Alloy Ethane MOF Metal Molecule TeO Cubic Propylene Chemistry Perovskite Acetylene DOBDC Syntheses Gas Glass Insulator Ionic
Sample state
Temperature Heat Situ Thermal Operate Room Time Pressure Frequency Process Density Ambient Reaction State Entropy
Electrolyte Power Voltage Dot Charge Ferroelectric Electrochemical Potential Capacity Technology Lithium Electric Energy Battery Cathode Storage Redox Cell Electrode Cycle Hysteresis Efficient
Units
Ms Mu Unit Angstrom
Elements
Mn Oxygen Fe Pb Iron Zn Ni Hydrogen Li Mg Co Ca Te Bi Sb Carbon Na
Solute Liquid Polar Adsorption Porous Host Interface Pore Surface Adsorb Layer
Techniques
Dynamic Proton Theoretical Spectroscopy Powder Pair Optics Bulk Theory Transport Crystallographic Synchrotron Refined Simulate Resolution Microscopy Phonon Resonant Laser Oriented Inelastic
Spin Fermion Chiral Exchange Topology RuCl Magnet Geometric Skyrmion Majorana Kitaev Orbit Band Ferromagnet Antiferromagnet Superconducting Interact Gap Quantum Excited Honeycomb Kagome
Composite Texture Manufacturing Stress Microstructure

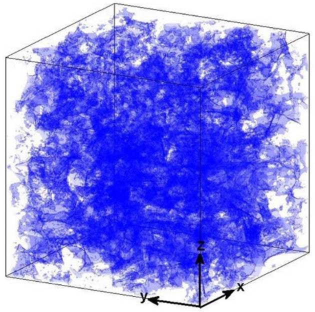


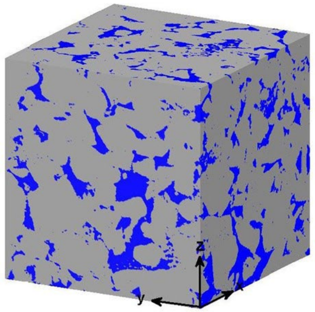
Energy & Environment

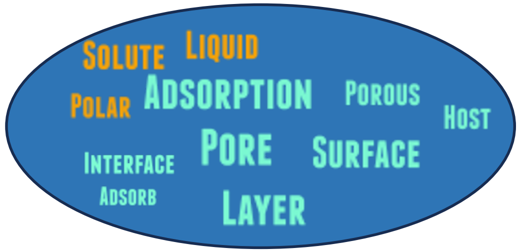






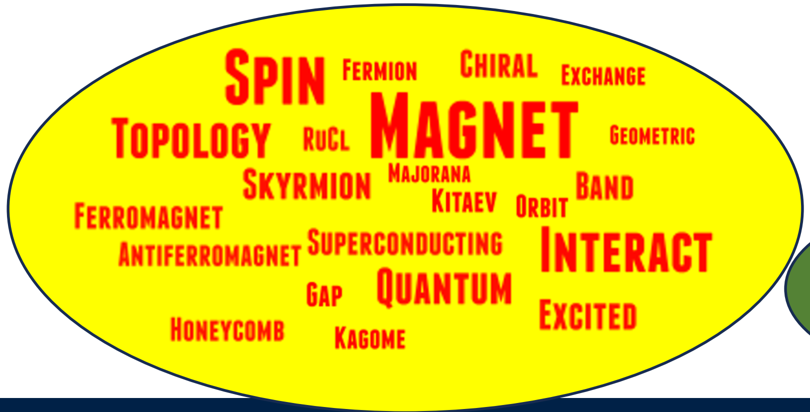


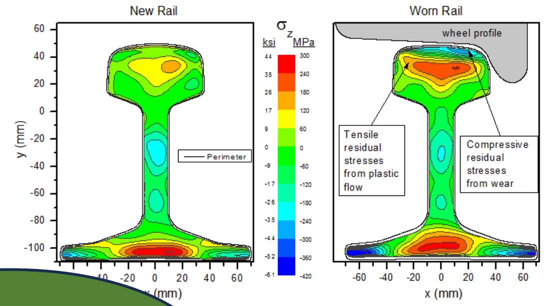


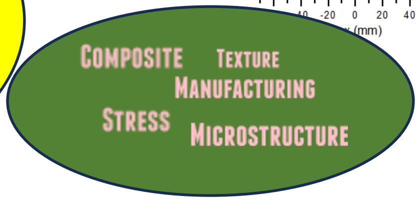


Heterogeneities, interfaces, disorder

Quantum Matter
Quantum Materials



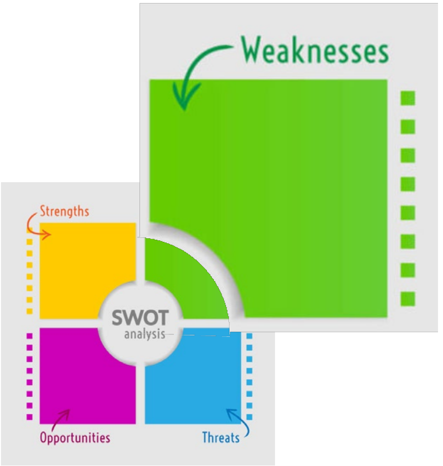




Engineering

Yes, but what about the next 25 years?

Quotes from SNS-STS workshop



”SNS-STS…will enable us to discover **fundamental properties of materials**” – *Paul Langan, ORNL*

“Without neutron scattering, we would know very little…about certain material systems like **superconductors and magnetic materials**” – *Efrain Rodriguez, U. Maryland*

”Understanding materials ‘**from the bottom up**’” – *Adrian Brugger, Columbia U.*

”…to remain **competitive and world-leading**’” – *Olivier Delaire, Duke U.*

”…broader spectrum of materials…**materials science and CMP…new states of matter**’” – *Stephen Wilson, UCSB*

”…**Solid-state chemistry**… **not so large crystals**’” – *Weiwei Xie, Luisiana State U.*

”…**Interfaces and heterostructures**… **predictably design** new materials” – *Laura Green, Florida State U.*

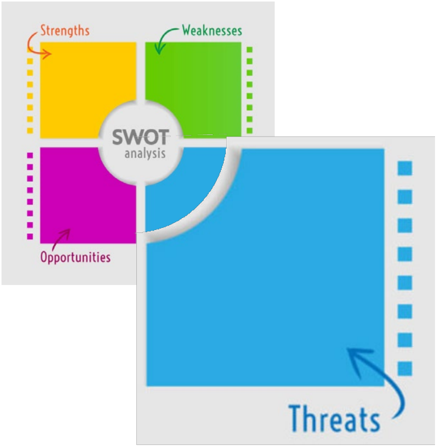
”…Fast time resolution information…**minutes or seconds**’” – *Claire White, Princeton*

”…vastly different **lengthscales…sub-nm to μm**…all in one shot’” – *Martin Mourigal, Georgia Tech*

Are neutrons coupled with the science of the future?

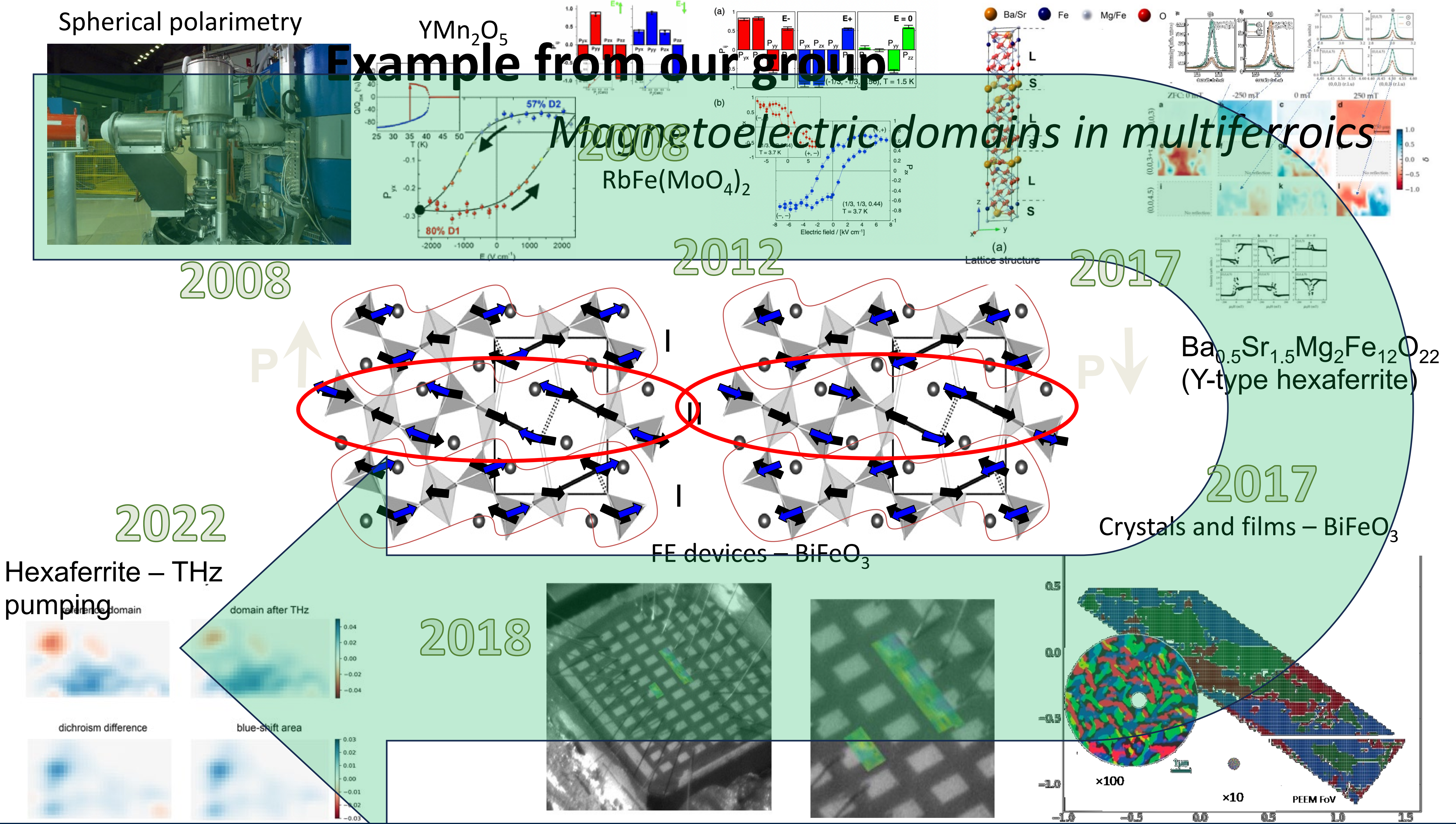
Science is moving on…

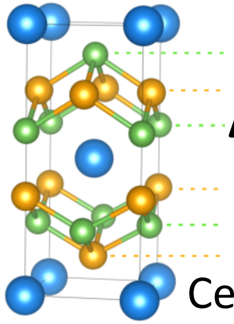
- …from bulk materials to devices (e.g., skyrmions, multiferroics…)
- …from 3D to 2D (VdW heterostructures, twisted graphene)
- …from Q-ω to the time and space domains



Example from our group

Magnetoelectric domains in multiferroics





$CeRh_2As_2$

Are neutrons coupled with the science of the future?

Results from ERC PE3 Consolidator panel – 11/23

E. Hassinger (MPI – Dresden) Exotic quantum states by locally-broken inversion symmetry in extreme conditions.

J. Herzen (T.U. Munich) Material Decomposition in X- ray Phase-Contrast Imaging with Coherent Sources

Nicola Poccia (Leibnitz-I – Dresden) 3D Cuprate Twistronics as a platform for high temperature topological superconductivity

Michael Sentef (U. Bremen) Cavity quantum materials

Basile Gallet (CEA) Physically-Based Ocean Transport

Amir Ariel (Weizmann) Biophysical Models of Bacterial Growth

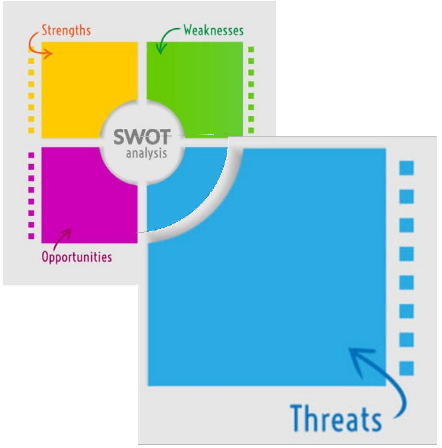
Yonatan Anahory (Jerusalem) Majorana zero mode control and detection platform

Moshe Ben Shalom (Tel Aviv) Switching Polytypes and Symmetries by Discrete vdW Sliding

Chase Broedersz (Vrjie U. Amsterdam) Learning the dynamic statistical folding of bacterial chromosomes

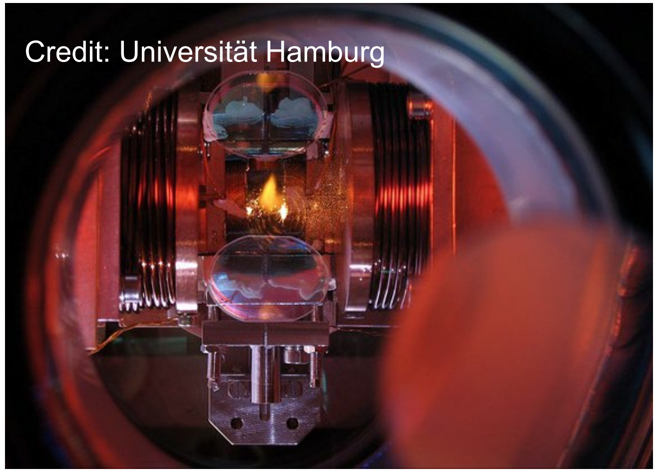
Lev Vidmar – (I. Josef Stefan) Boundaries of quantum chaos

Chiara Ciccarelli (Cambridge) Picosecond superconductivity-driven spin-torques



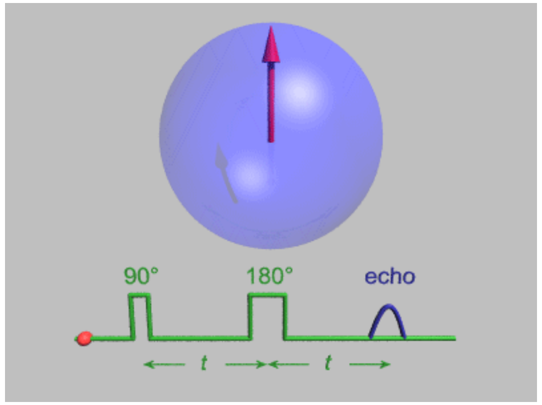
Many opportunities but no low-hanging fruits

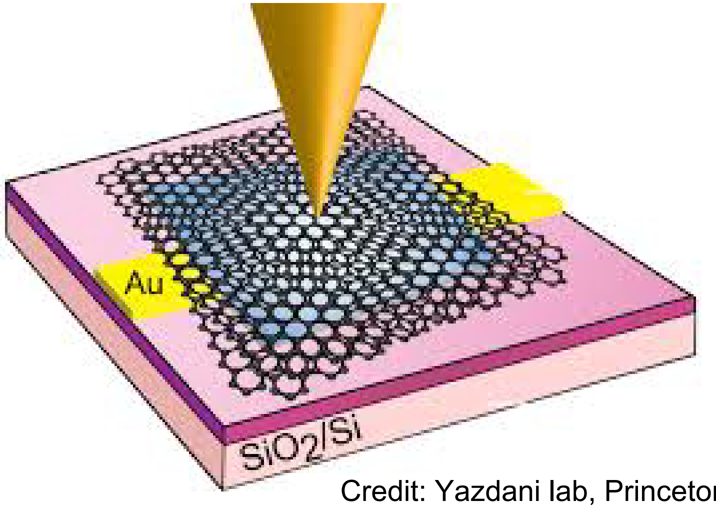
Can neutrons do something in…?



Non-equilibrium many-body phases (e.g., time crystals)

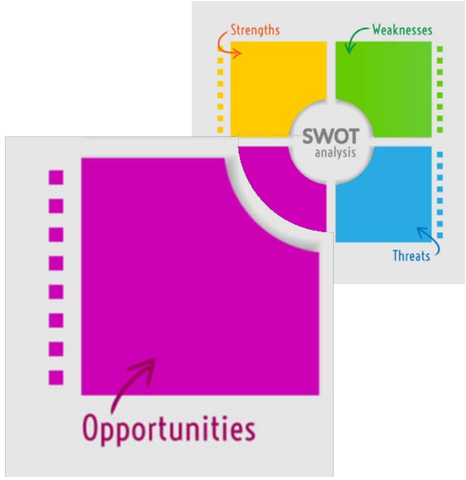
Radically new techniques (e.g., Spin Echo in the 1970s)

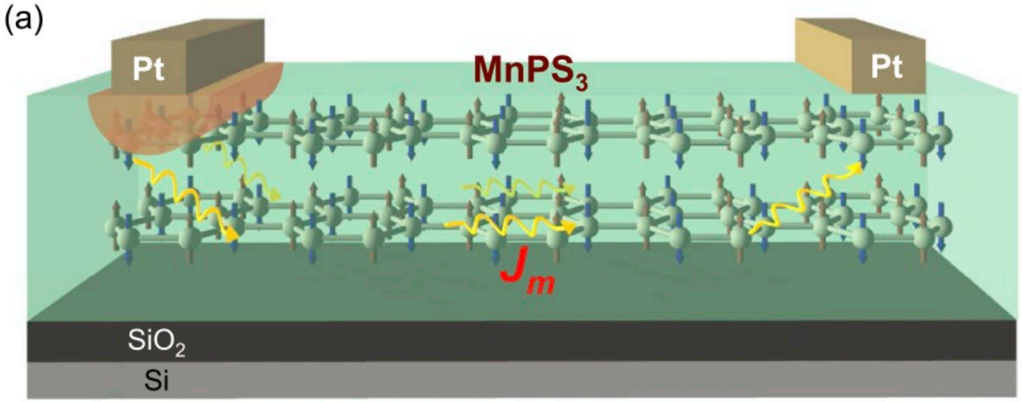




Credit: Yazdani lab, Princeton

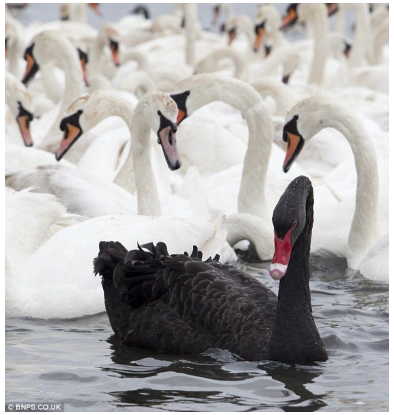
'Twistronics'





Structure & dynamics in 2D magnets

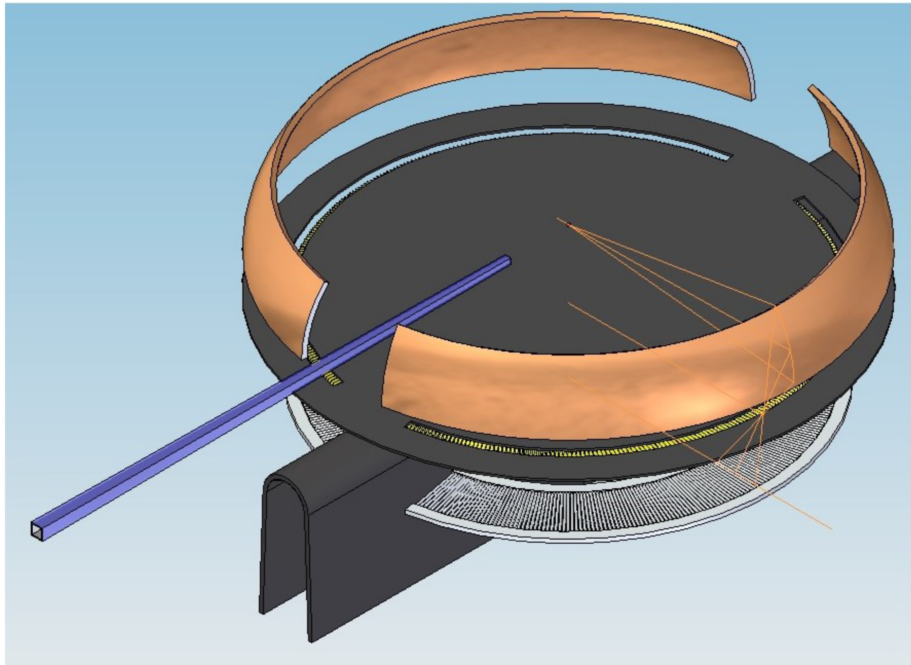
Credit: W. Xing *et al.*, PRL 2019



‘Black swan’ instruments

lessons from neutrons…

& synchrotron



Mushroom (ISIS-Endeavour)

I22-RIXS @ Diamond

Manipulating neutron polarization (e.g., D3, IN20, cryopad).

BIFROST (ESS)

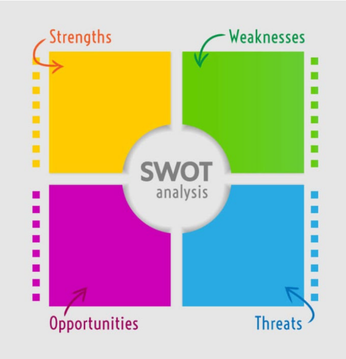
NEUTRONS FOR SOCIETY

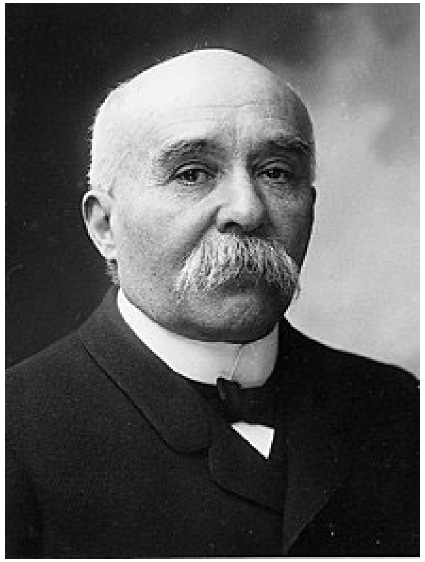
And finally….

A few pearls of wisdom

Work on something that will make money or else something that will interest theorists

Bell Labs Management





Generals always prepare to fight the last war, especially if they had won it.

Georges Clemenceau

Thank you for listening