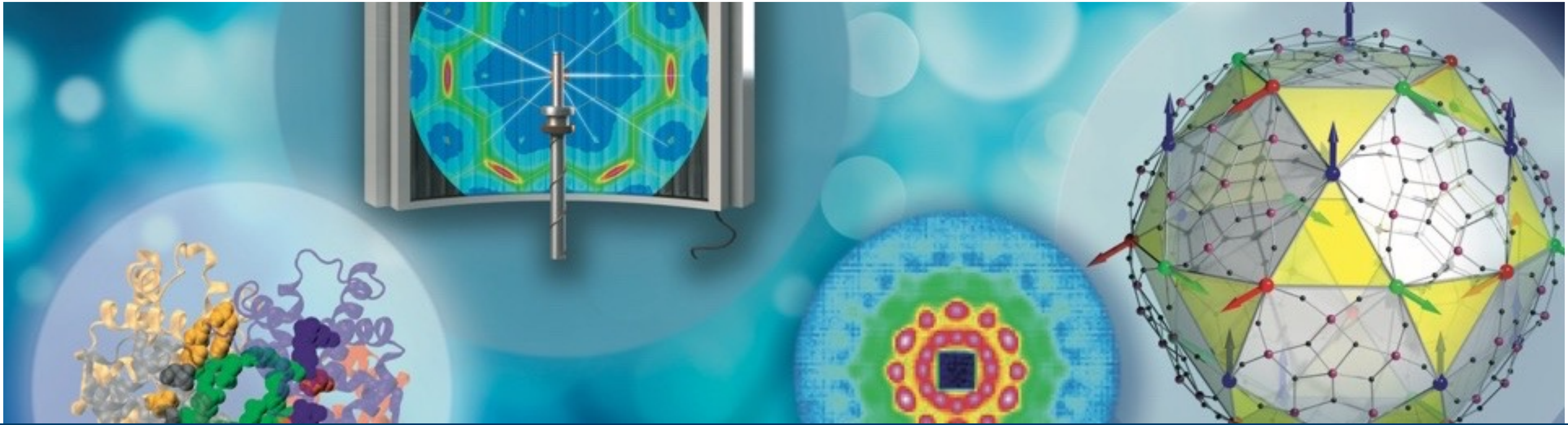


NEUTRONS FOR A SUSTAINABLE FUTURE

Societal Challenges, Science with Neutrons & Facilities

1 MARCH 2023 I THOMAS BRÜCKEL; JÜLICH CENTRE FOR NEUTRON SCIENCE

JÜLICH Forschungszentrum Shaping Change

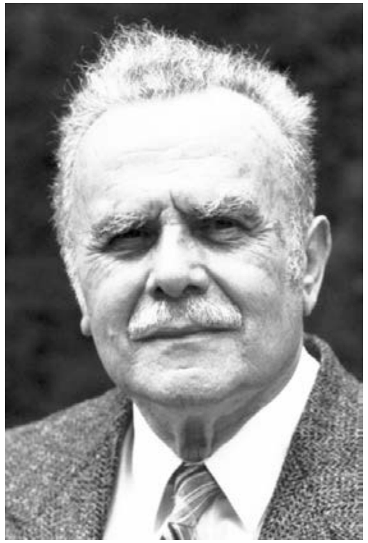
NEUTRONS: A SPECIAL GIFT FOR SCIENCE

Essential Probe to Understand and Engineer Materials

The Nobel Prize in Physics 1994 was divided equally between Bertram N. Brockhouse "for the development of neutron spectroscopy" and Clifford G. Shull "for the development of the neutron diffraction technique."

from: NobelPrize.org

Clifford G. Shull



Bertram N. Brockhouse

Cliff Shull:

„Neutrons tell us where the atoms are and how they move.“

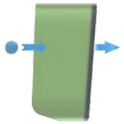
NEUTRONS: WHAT MAKES THEM SO SPECIAL?

Essential Probe to Understand and Engineer Materials

Strength of neutrons

light elements, isotopic labelling
H, D, Li, Na,…

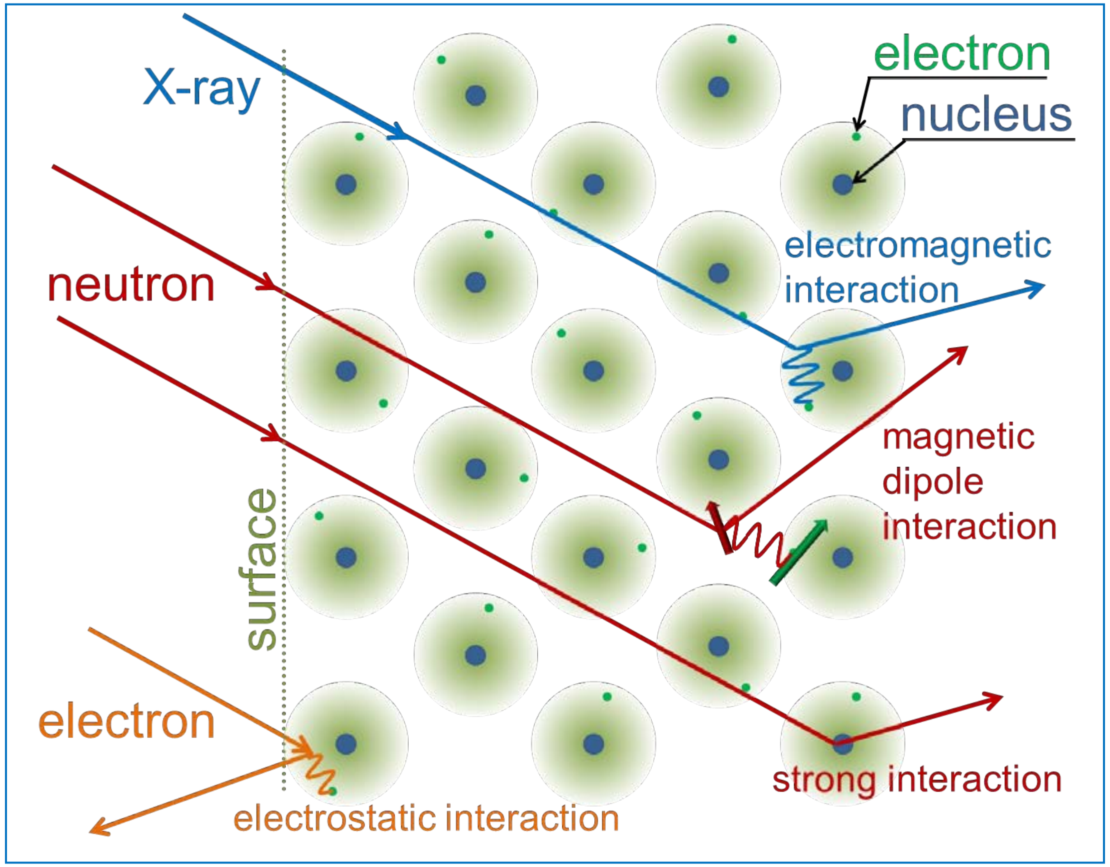
gentle probe
nondestructive



penetrating

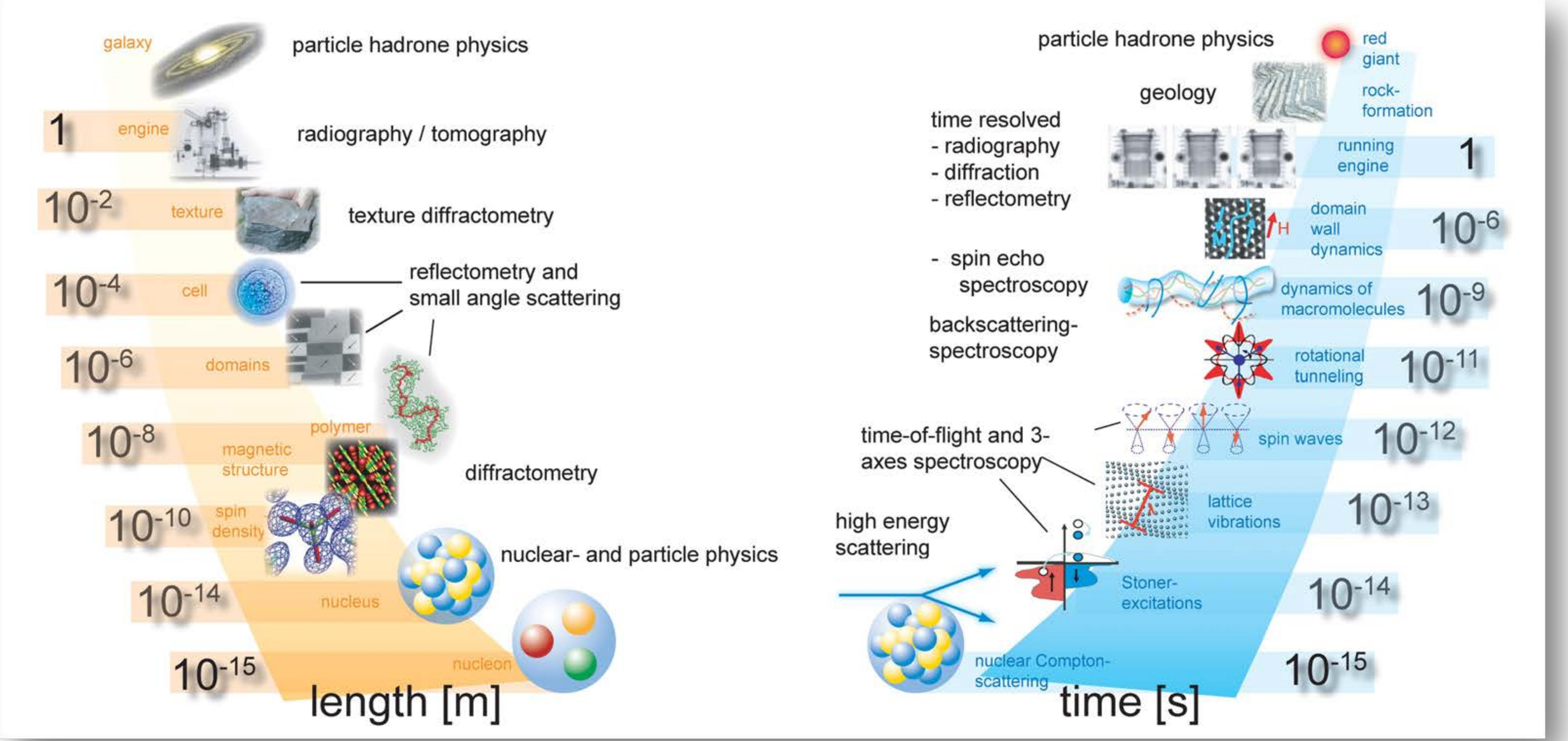
magnetism
spin

dynamics



neutrons, **X-rays** and **electrons** have different interactions with atoms
together they provide important complementary structural information

NEUTRONS: LENGTH AND TIME SCALES



neutrons cover length scales from picometer to meter and time scales from femtoseconds to hours

OUTLINE

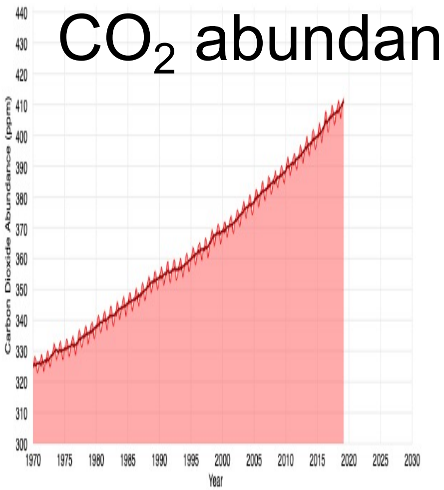
CLIMATE CRISIS

A huge thread to human civilization on the planet

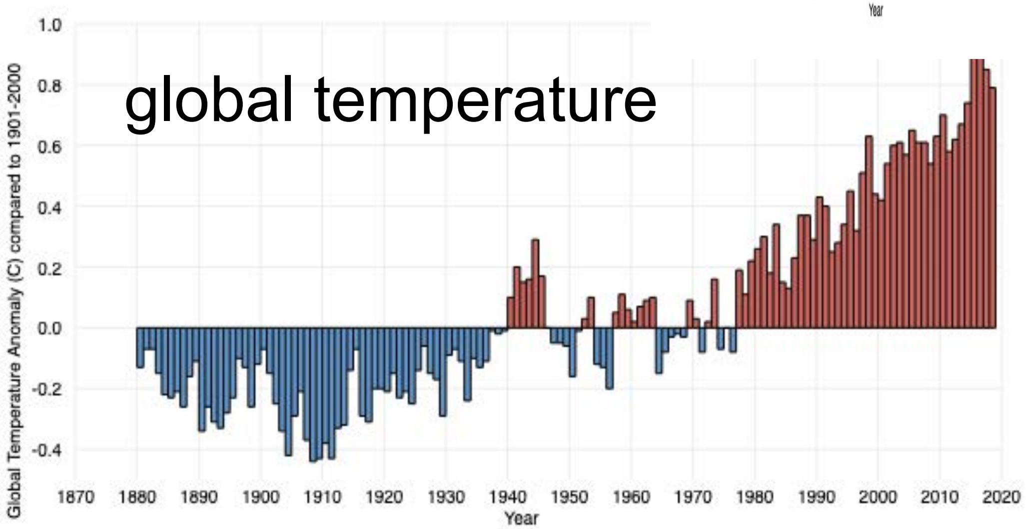
National Oceanic and Atmospheric Administration
U.S. Department of Commerce

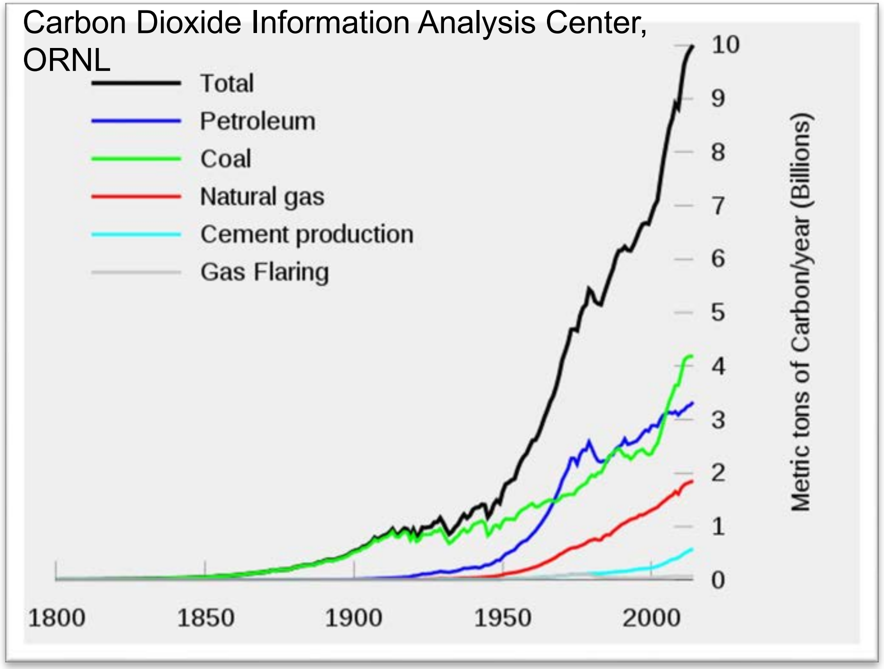
Climate.gov
science & information for a climate-smart nation

CO_2 abundance



global temperature





global carbon emission

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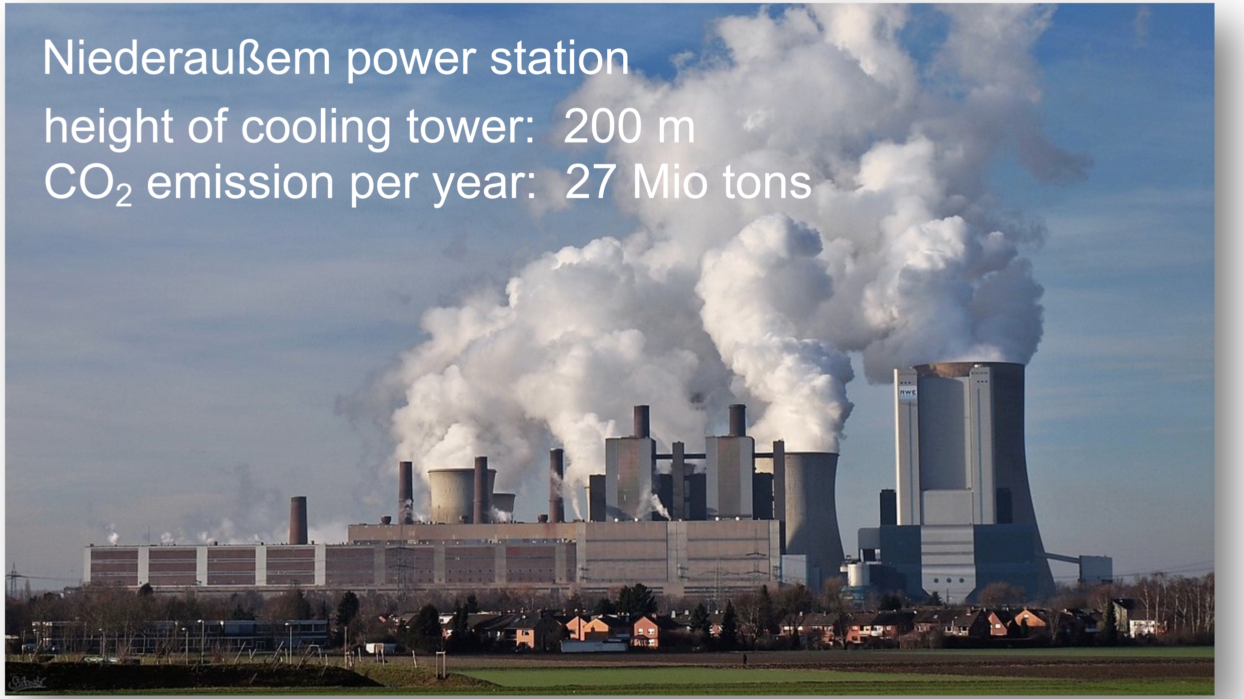
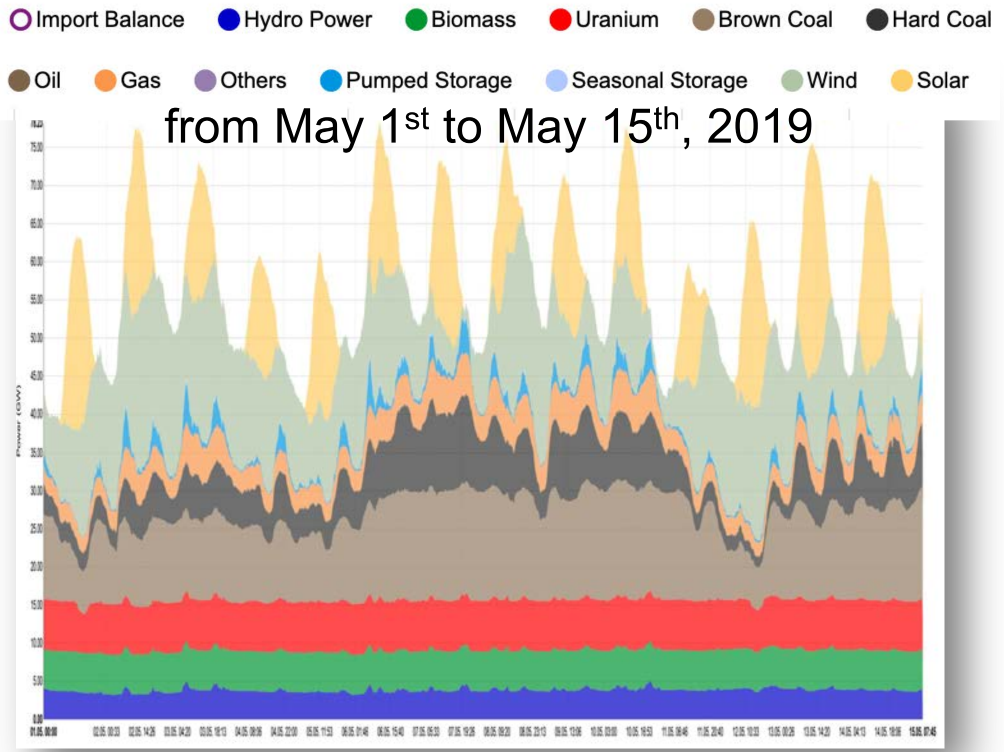
CLIMATE CHANGE & ENERGY TRANSITION

Electricity production: From fossil to renewable energies



problem with fossil fuels (here: lignite)



problem of renewable energies (wind, solar)

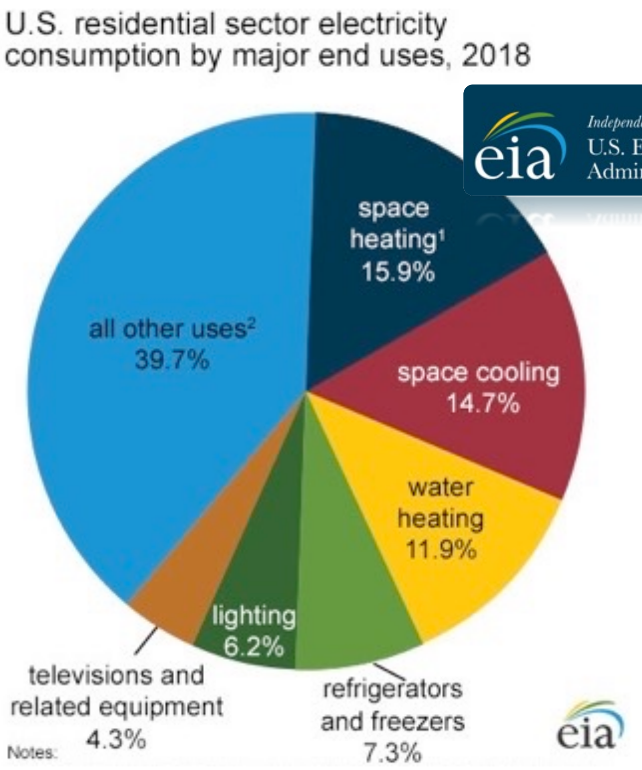
→ energy conversion & storage: a materials problem!

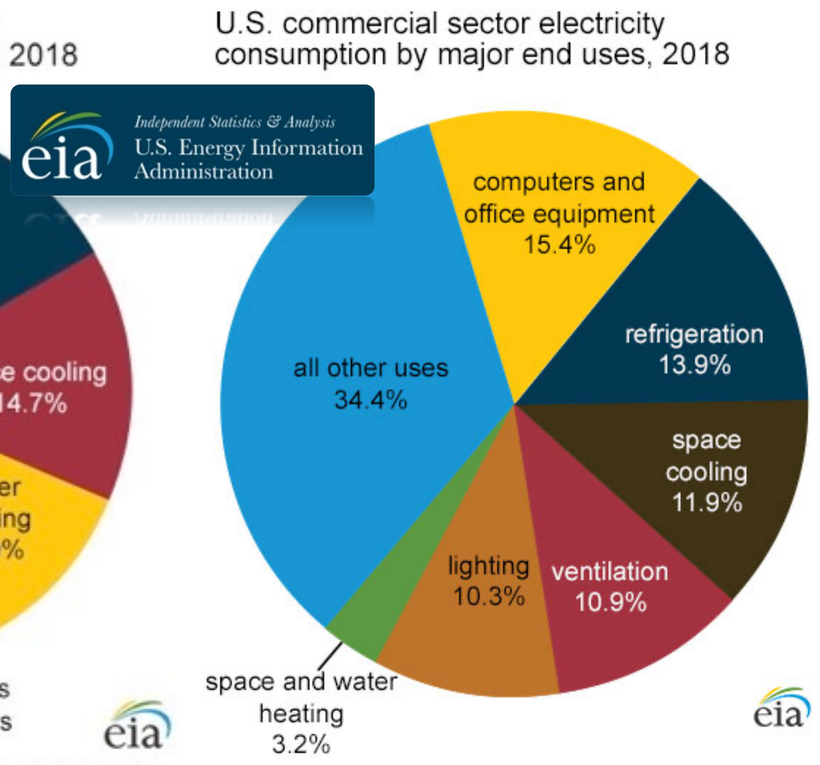
JCNS Jülich Centre for Neutron Science

JÜLICH Forschungszentrum

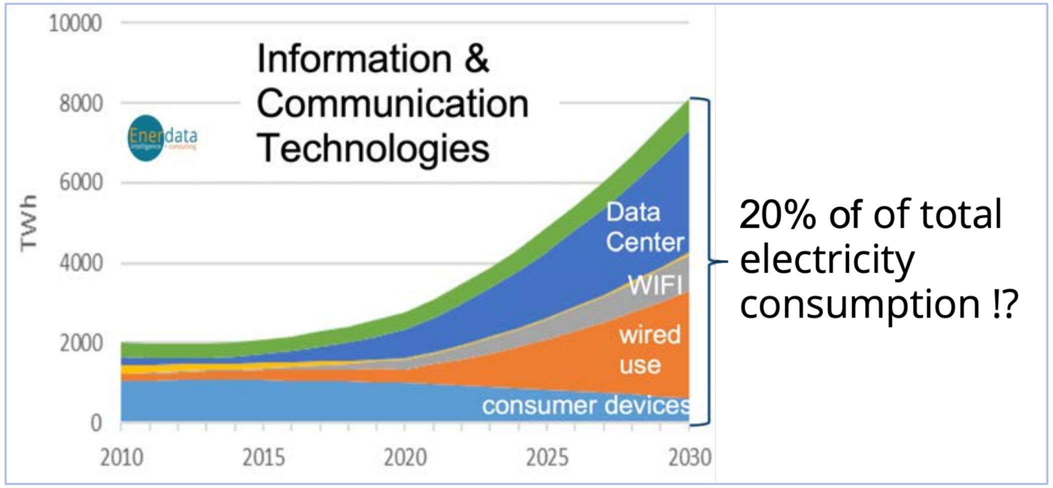
THE ENERGY TRANSITION

The other side of the medal: electric energy consumption





Source: U.S. Energy Information Administration, *Annual Energy Outlook 2019*, Table 5, January 2019



cooling: about ¼ of electric energy consumption

ICT’s: growth in electric energy consumption

→ energy saving: a materials problem!

OUTLINE

- Grand Challenge: Climate Crisis & Energy Transition
- **Neutrons: Essential Tool for Energy Research – Batteries**
- Neutrons: Essential Tool for Energy Research – Cooling
- Neutrons: Essential Tool for Energy Research & Information Technologies
- Neutrons: Essential Tool for Health Research
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- Summary

LITHIUM-ION RECHARGEABLE BATTERIES (LIBS)

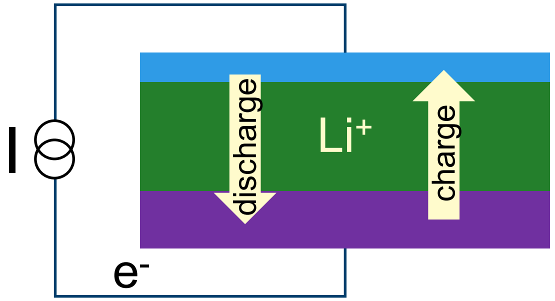
Conventional: powerful but dangerous!

- highest energy density in terms of specific energy (Wh kg^{-1}) and volumetric energy density (Wh L^{-1}).
- liquid electrolytes are intrinsically volatile and flammable.

→ all-solid-state LIB‘s for portable devices

ALL-SOLID-STATE, THIN FILM LIB BATTERIES

Si–Li_3PO_4–$LiCoO_2$ batteries: Degradation during charge & discharge cycles



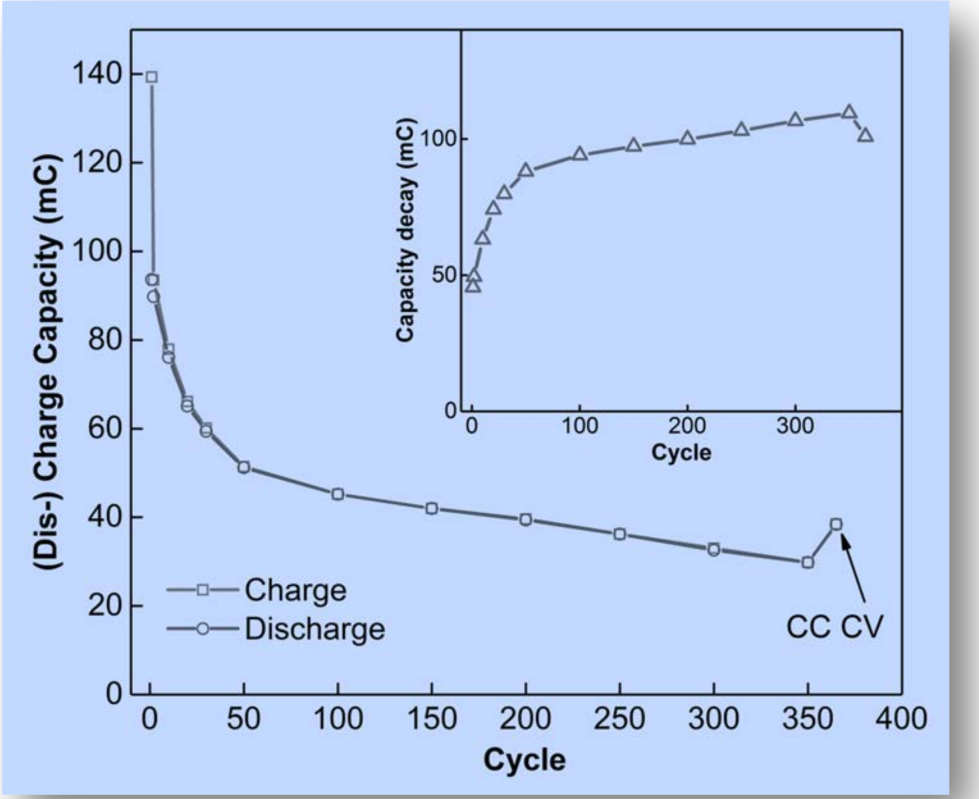
Si anode (50 nm)

Li_3PO_4 electrolyte (2000 nm)

$LiCoO_2$ cathode (550 nm)

$$LiCoO_2 \underset{\text{Discharge}}{\overset{\text{Charge}}{\rightleftarrows}} Li_{1-x}CoO_2 + xLi^+ + xe^-$$

$$Li_ySi \underset{\text{Discharge}}{\overset{\text{Charge}}{\leftrightarrows}} yLi^+ + ye^- + Si$$



➢ dramatic loss of capacity with charging and discharging cycles; origin of degradation?

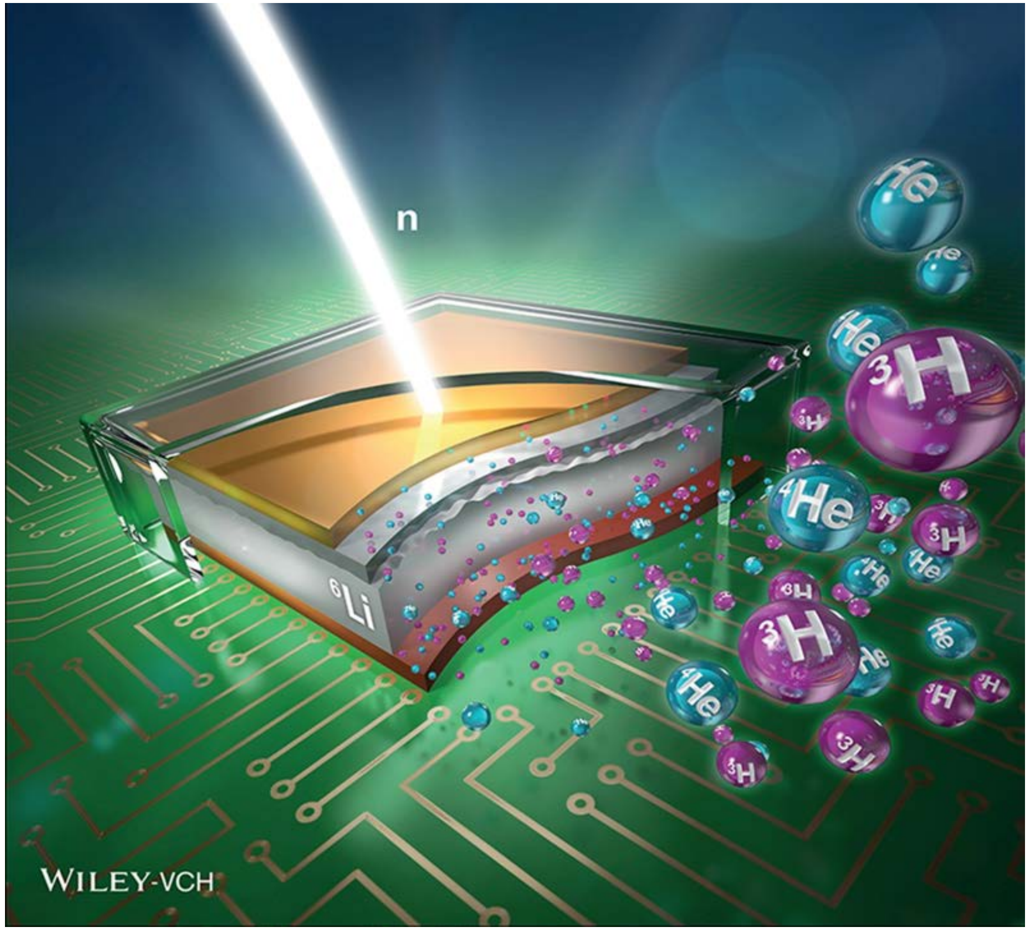
C. Chen, et al.; Adv. Energy Mater. 8 (2018),1801430 / DOI: 10.1002/aenm.201801430

NEUTRONS: ESSENTIAL TOOL FOR ENERGY RESEARCH

Energy Revolution: Fuel Cells & Batteries → Light Elements → Neutrons!

- Neutron Depth Profiling (NDP)
- Neutron absorption: $n + 6Li \rightarrow {}^{4}He + 3H$
- **α**-particles with 2727 keV and triton with 2055 keV initial energy lose energy through collisions depending on the depth of formation and the material penetrated

→ depth sensitive probe for ^{6}Li



C. Chen, et al.; Adv. Energy Mater. 8 (2018),1801430 / DOI: 10.1002/aenm.201801430

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NEUTRONS: ESSENTIAL TOOL FOR ENERGY RESEARCH

Neutron Depth Profiling (NDP): powerful operando method!

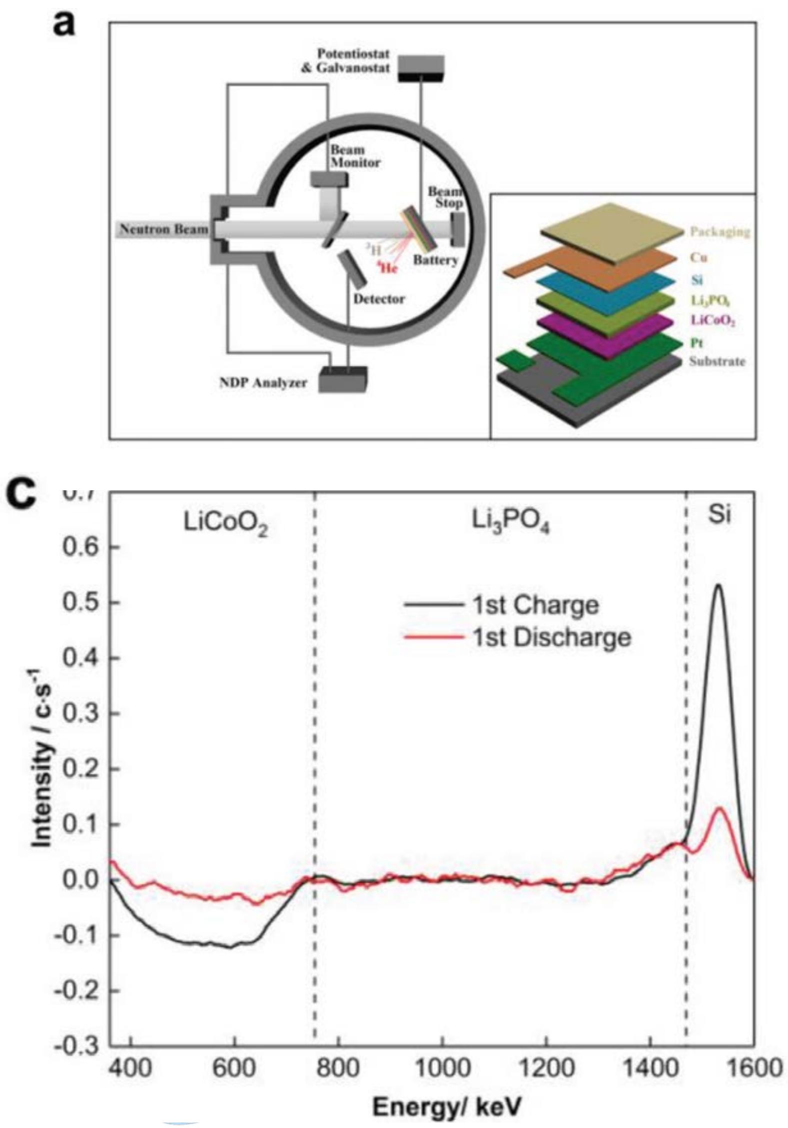
- Charging:

  Li^+: $LiCoO_2$ cathode → Si anode

- Discharging:

  only partly reversible;

  Li layer forming at anode / electrolyte interface



C. Chen, et al.; Adv. Energy Mater. 8 (2018),1801430 / DOI: 10.1002/aenm.201801430

NEUTRONS: ESSENTIAL TOOL FOR ENERGY RESEARCH

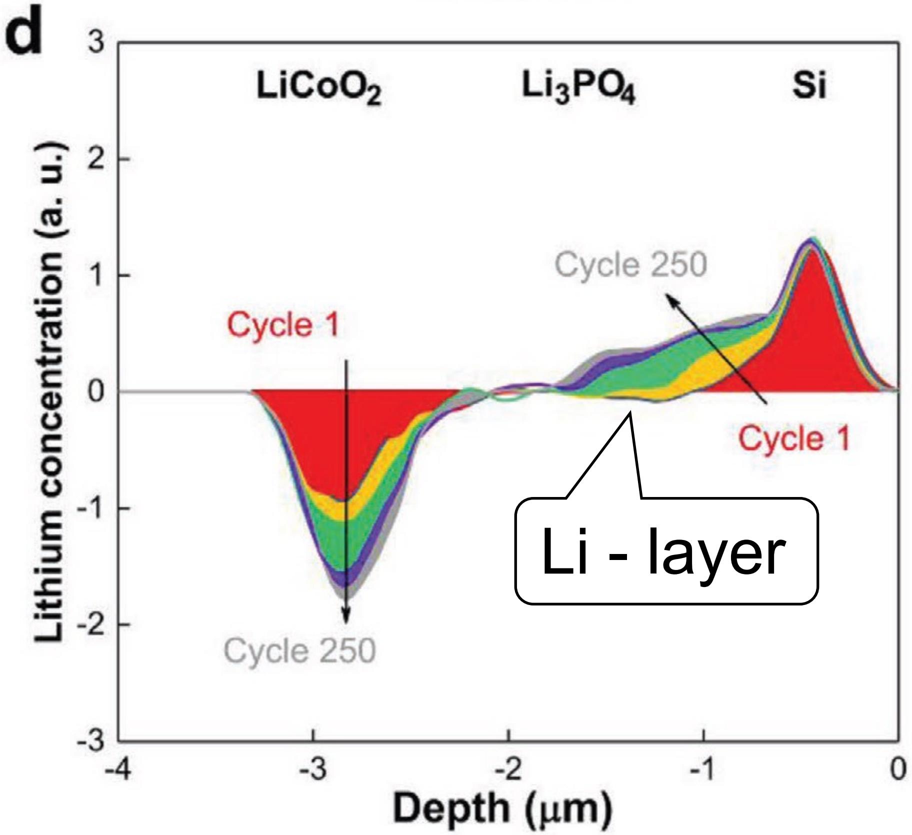
NDP reveals Li immobilization layer

- cycling:

  a growing Li-immobilization layer is formed between the Si anode and the solid electrolyte

- complementary Si-mapping with EDX (Elemental energy dispersive X-ray spectroscopy)

  → Si enrichment in imobilization layer



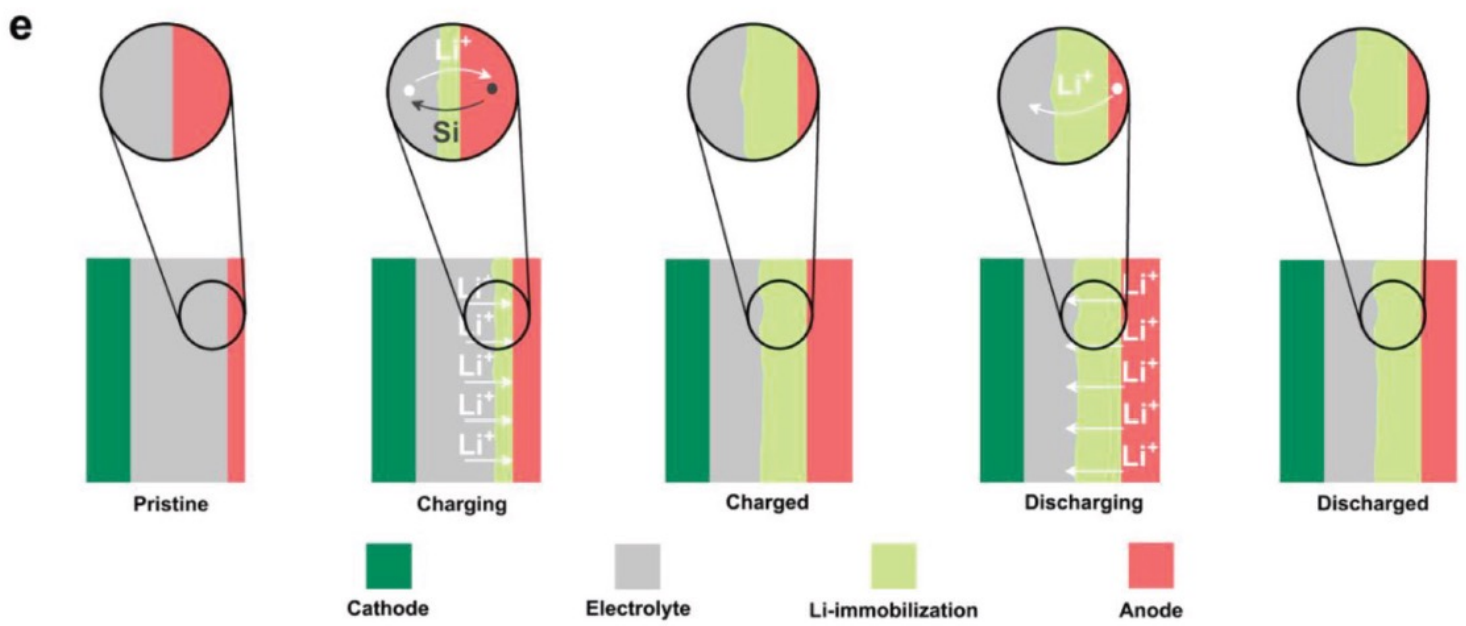
C. Chen, et al.; Adv. Energy Mater. 8 (2018),1801430 / DOI: 10.1002/aenm.201801430

NEUTRONS: ESSENTIAL TOOL FOR ENERGY RESEARCH

Li-immobilization layer developing at anode / electrolyte interface

- new phase formed at electrolyte / anode interface during cycling
- Li-immobilization is induced by Si-migration into the solid-state electrolyte under current flow

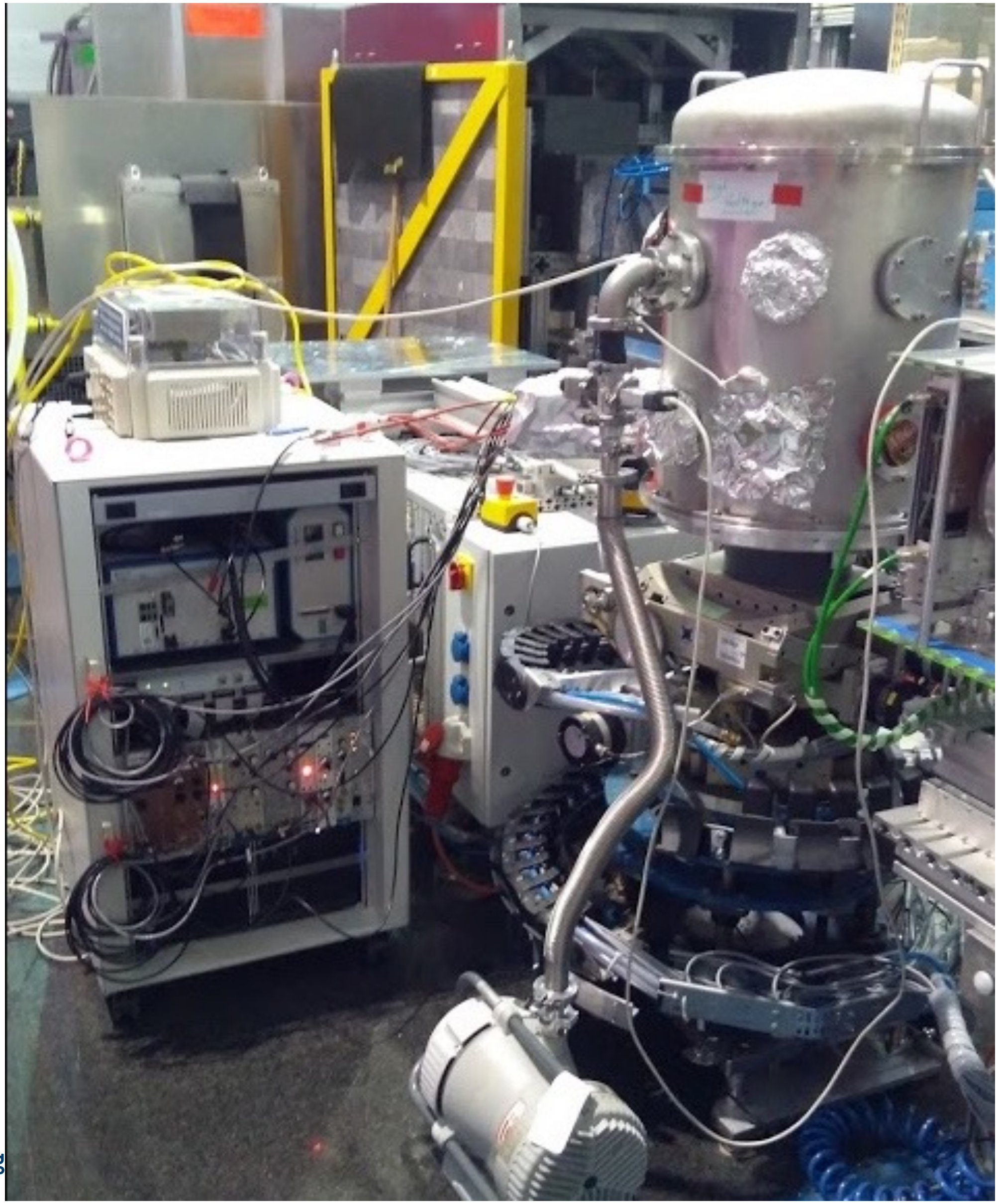
→ introduce specific protective layers between Si and Li_3PO_4, which function as barrier for Si-migration

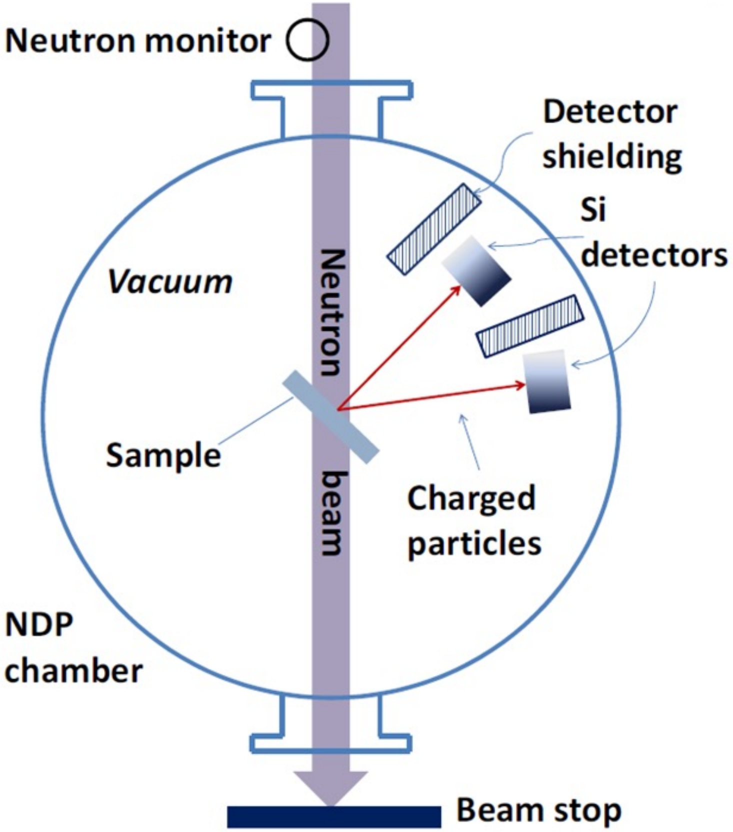


Neutrons (here operando NDP) reveal degradation mechanism
→ interfacial modifications to improve battery performance

C. Chen, et al.; Adv. Energy Mater. 8 (2018),1801430 / DOI: 10.1002/aenm.201801430

NDP CHAMBER OF JCNS @ MLZ





E. Vezhlev, et al.; Radiation Effects and Defects in Solids 175 (2020), 342
DOI:10.1080/10420150.2019.1701466

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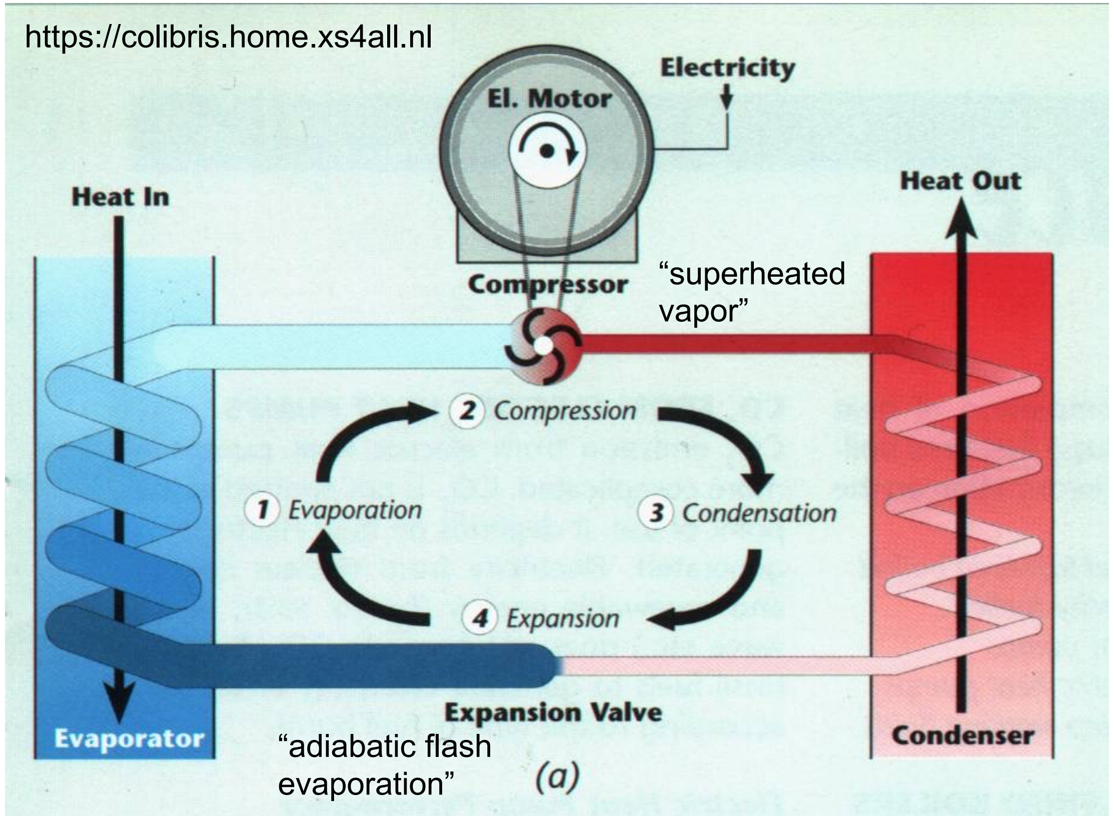
VAPOR COMPRESSION CYCLE REFRIGERATION

todays standard (since about 200 years !!!)



heat-pump:

based on the entropy change during compression and expansion of gases

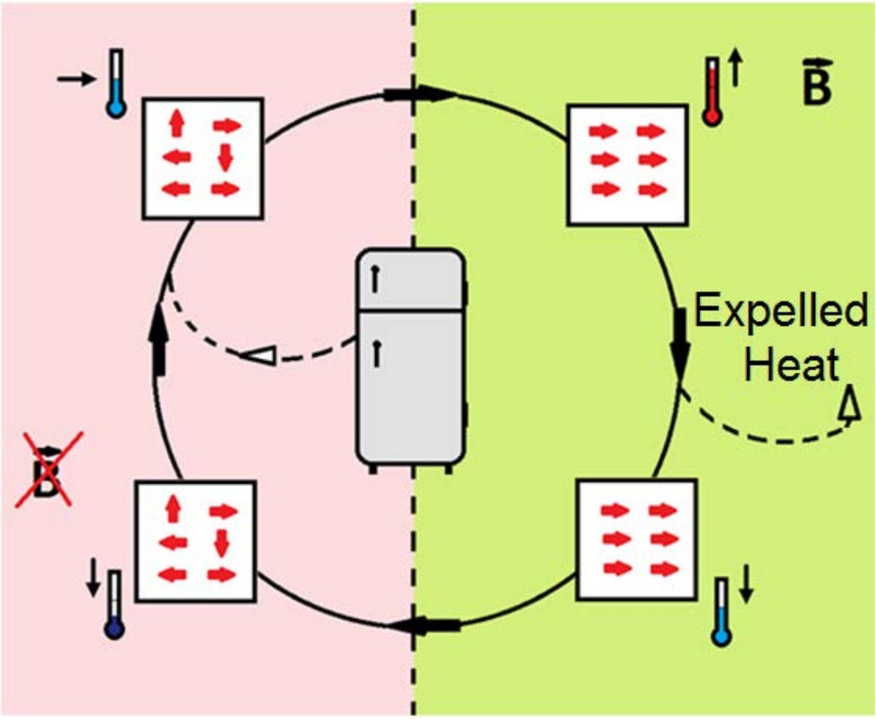
refrigerant, e.g. "FREON"

(du Pont trademark for chlorodifluoromethane)

ozone depletion, climate active

CAN WE DO BETTER? YES: MAGNETOCALORIC COOLING!

potential energy saving of up to 30%; without hazardous gases!



based on the entropy change during application and removal of a magnetic field on a magnetic material

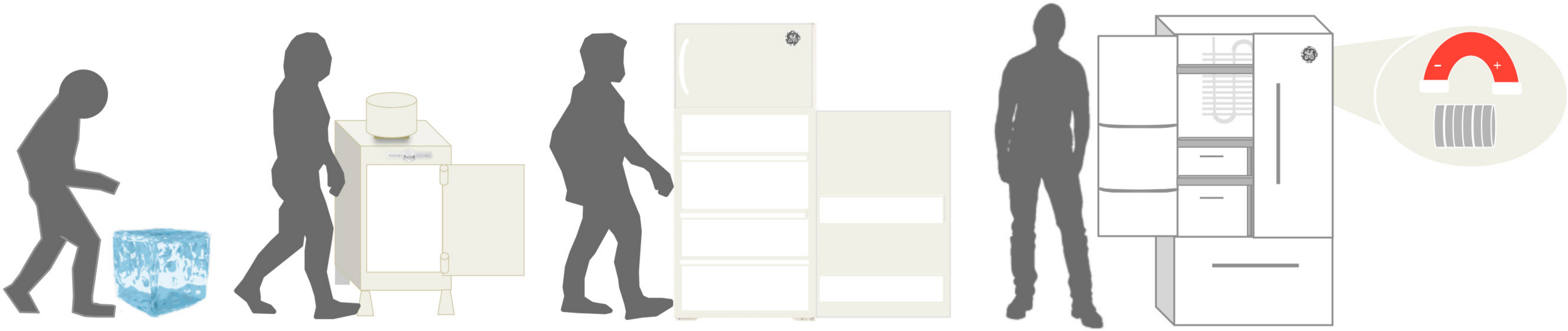
✓ potential energy saving of up to 30%

[K. A. Gschneidner Jr. et. al., Int. J. Refrig. 31, 945 (2008)]

THE OPTIMISTIC VIEW OF A BIG COMPANY

GE APPLIANCES
a Haier company

The evolution of refrigeration...



1000 B.C.
Ice harvesting

1927
GE 's first electric powered refrigerator

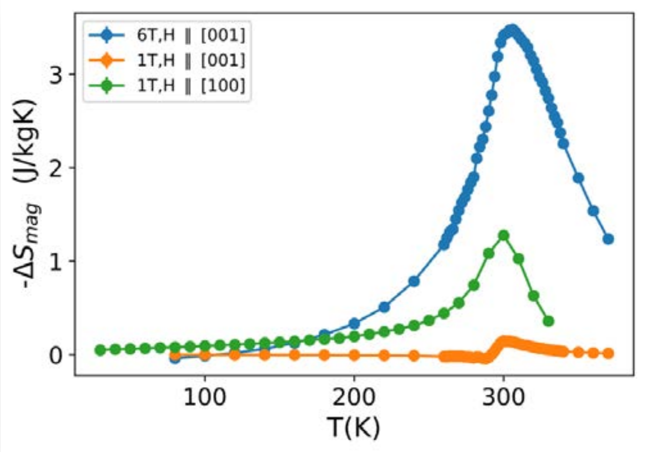
1927 - Today
Vapor compression technology dominates home refrigeration

2020
GE expects magnetic refrigeration to be 20 percent more efficient and replace compressor technology in homes

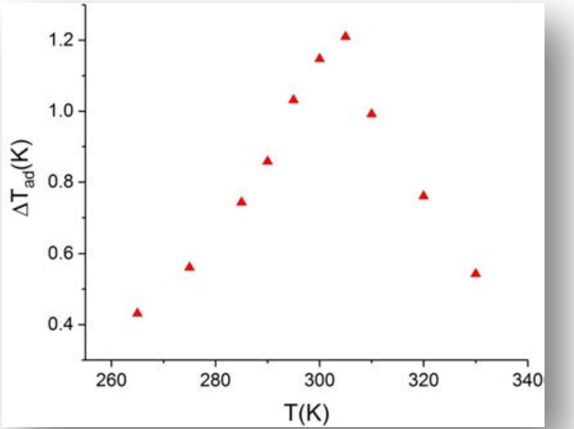
THE $Mn_{5-x}Fe_xSi_3$ SERIES

neutrons reveal microscopic mechanism of magnetocaloric effect

entropy change (anisotropic)



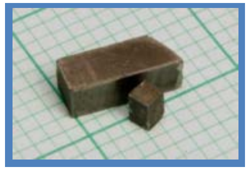
temperature change for 2T



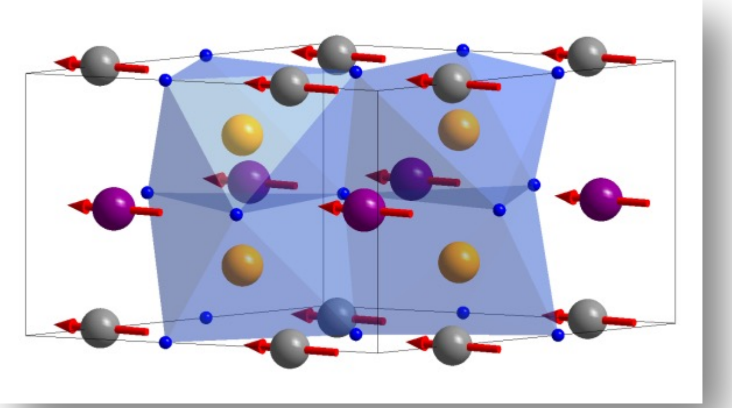
Nour Maraytta et. al., Journal of Alloys and Compounds 805 (2019), 1161

$MnFe_4Si_3$:

- ✓ modestly large MCE ≈ 2.1J/kg K at ΔB=0-2T
- ✓ T_c=299.6(1.0) K in the interesting range
- ✓ good molding and processing behavior, mechanically stable
- ✓ abundant, cheap and environ-mentally friendly constituents
- ✓ we could grow single x-tals!

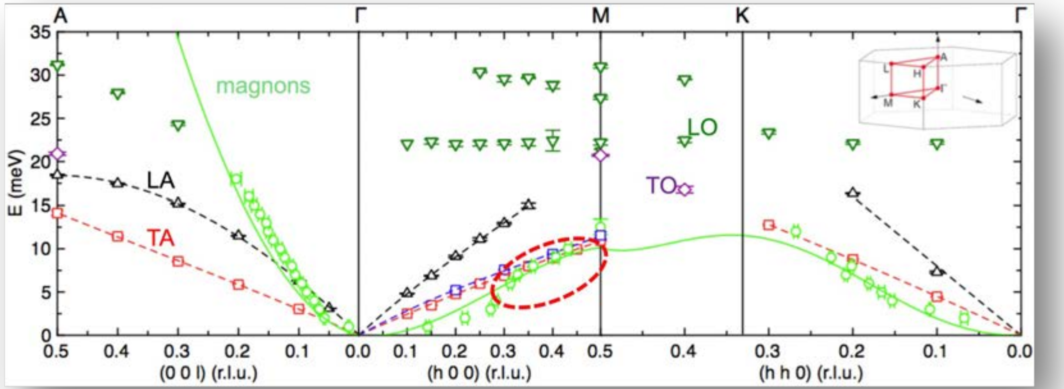


neutrons: magnetic structure



Hering et. al., Chem. Mat. 27 (2015), 7128

neutrons: lattice and magnetic excitations



N. Biniskos et al., Phys. Rev. B 96 (2017), 104407 & Phys. Rev. B 105 (2022),104404

Neutrons give access to the microscopic mechanism of entropy change

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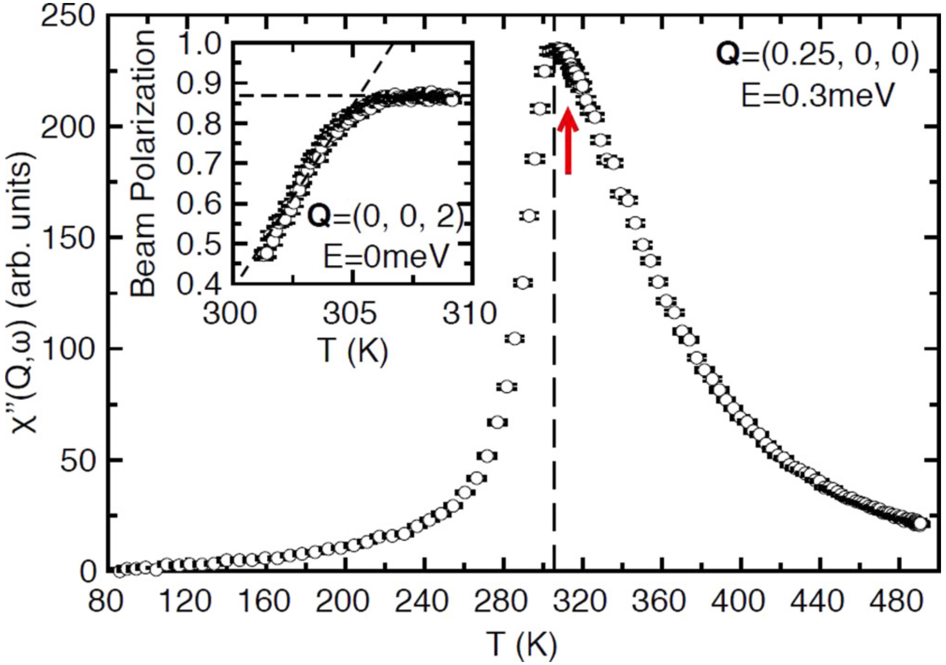
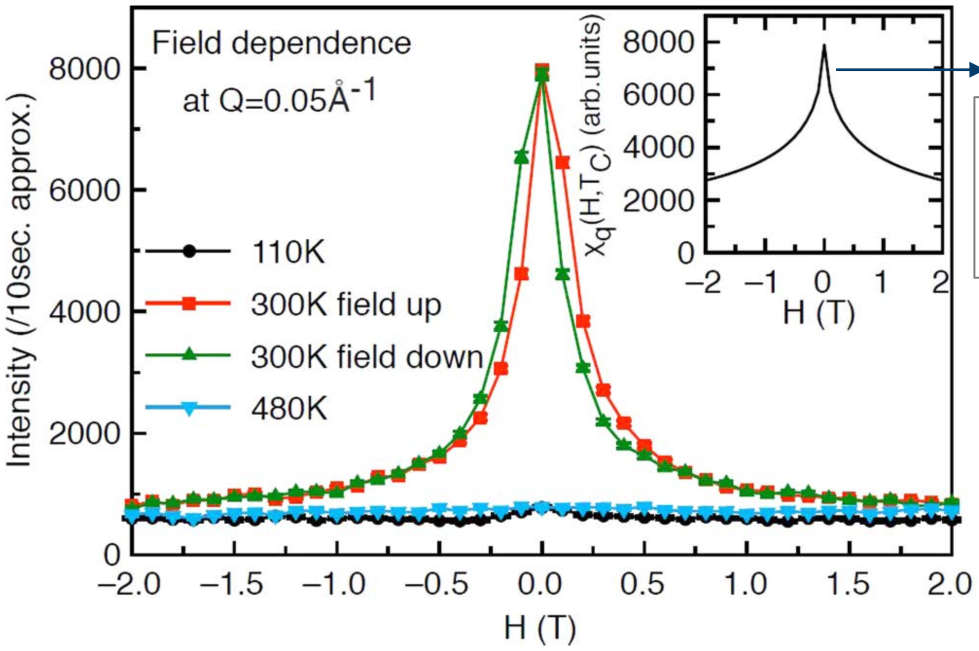
PARAMAGNETIC SCATTERING $MnFe_4Si_3$

instable magnetic moment → enhanced MCE at magnetic phase transition FM → PM

dynamical susceptibility:



field dependence for E=0:



Landau theory:

$$\chi_q^{\parallel}(H,T_C) = \frac{\chi_q(0,T_C)}{1+\left(\frac{27}{30}\right)^{1/3}\left(\frac{\kappa_0}{q}\right)^2\left(\frac{g\mu_B H}{k_B T_C}\right)^{2/3}}$$

$$\chi_q^{\perp}(H,T_C) = \frac{\chi_q(0,T_C)}{1+\left(\frac{1}{30}\right)^{1/3}\left(\frac{\kappa_0}{q}\right)^2\left(\frac{g\mu_B H}{k_B T_C}\right)^{2/3}}.$$

- ✓ strong field dependence: 2T field suppresses magnetic fluctuations
- ✓ suppression much stronger than predicted by Landau theory
- ✓ instable magnetic moment → MCE effect → recipe for enhancement

N. Biniskos et al., Phys. Rev. B 96 (2017), 104407
F.J. dos Santos et al., Phys. Rev. B 103 (2021), 024407
N. Biniskos et al., Phys. Rev. B 105 (2022),104404

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TOPOLOGY IN CONDENSED MATTER PHYSICS

The Nobel Prize in Physics 2016

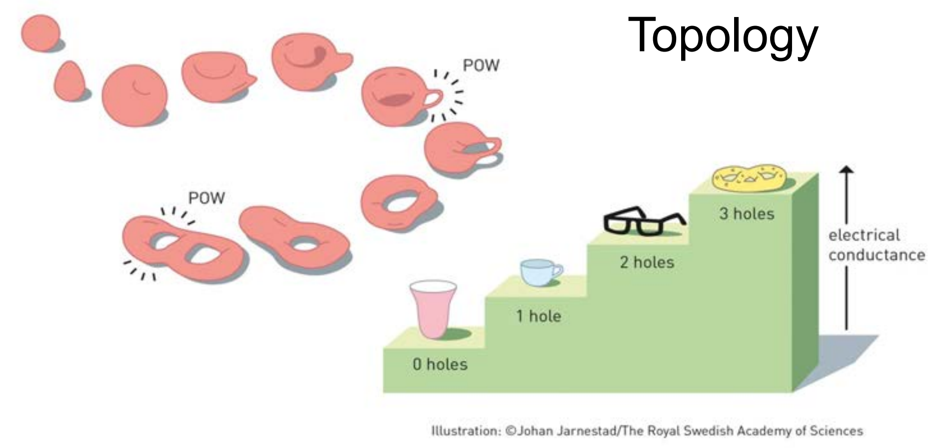
© Nobel Media AB. Photo: A. Mahmoud
David J. Thouless
Prize share: 1/2

© Nobel Media AB. Photo: A. Mahmoud
F. Duncan M. Haldane
Prize share: 1/4

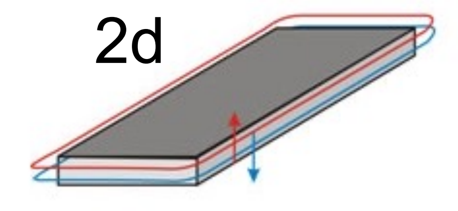
© Nobel Media AB. Photo: A. Mahmoud
J. Michael Kosterlitz
Prize share: 1/4

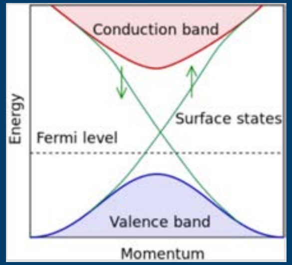
nobelprize.org

The Nobel Prize in Physics 2016 was awarded with one half to David J. Thouless, and the other half to F. Duncan M. Haldane and J. Michael Kosterlitz "for theoretical discoveries of topological phase transitions and topological phases of matter"



Topological insulators:





insulating bulk, conducting surface states, e.g. Bi_2Se_3

TWO DIMENSIONAL MATERIALS

The Nobel Prize in Physics 2010

© The Nobel Foundation. Photo: U. Montan

Andre Geim

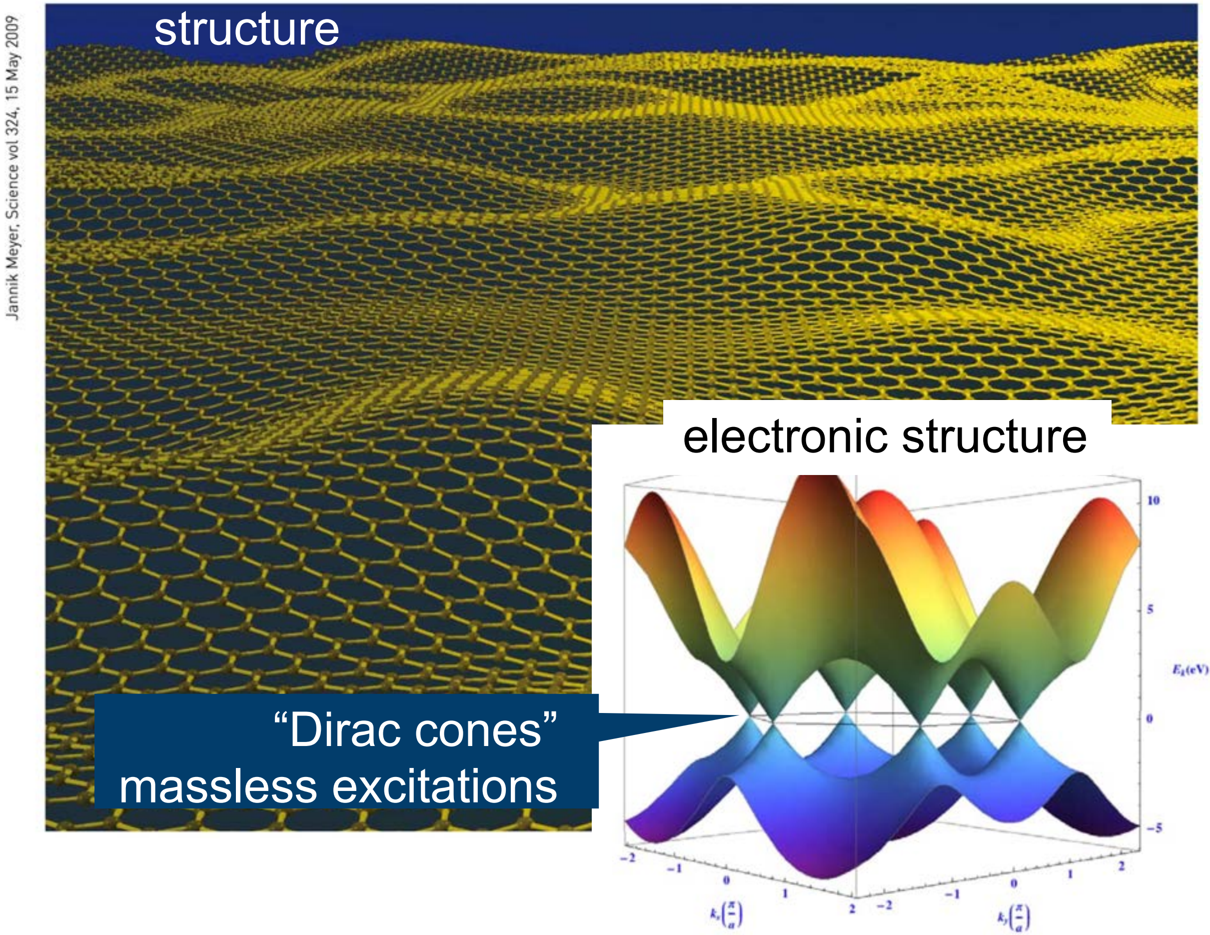
Prize share: 1/2

© The Nobel Foundation. Photo: U. Montan

Konstantin Novoselov

Prize share: 1/2

The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov "for groundbreaking experiments regarding the two-dimensional material graphene"



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SPINTRONICS

The Nobel Prize in Physics 2007

Albert Fert

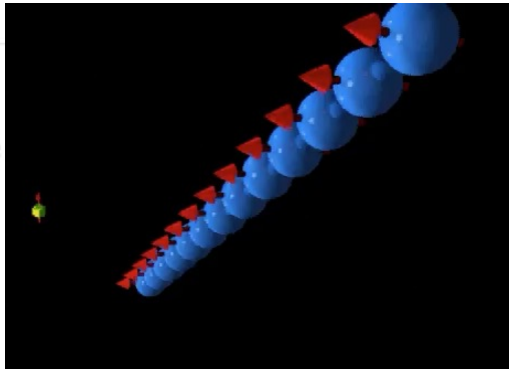
Prize share: 1/2

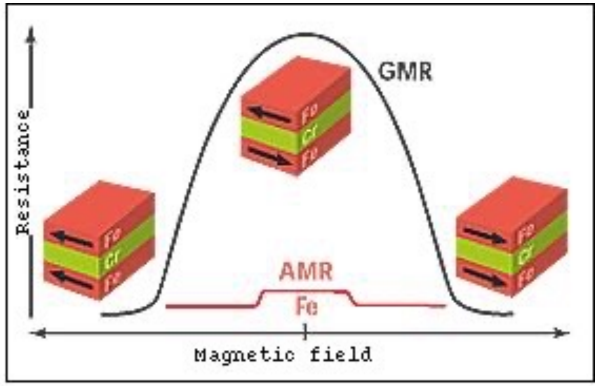
Peter Grünberg

Prize share: 1/2

The Nobel Prize in Physics 2007 was awarded jointly to Albert Fert and Peter Grünberg "for the discovery of Giant Magnetoresistance"

nobelprize.org





birth of SPINTRONICS:
Information transport, storage and processing (IT) using the spin of the electron

→ MAGNONICS:
IT using spin waves (magnons): no electric current, wavelengths in the nanometer range & GHz frequencies, → downscaling & high clock frequencies

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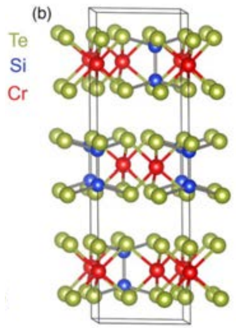
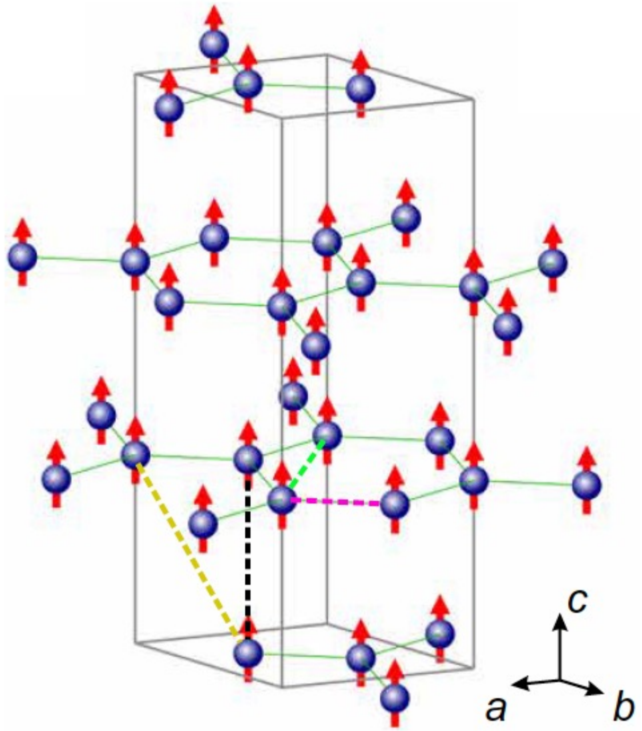
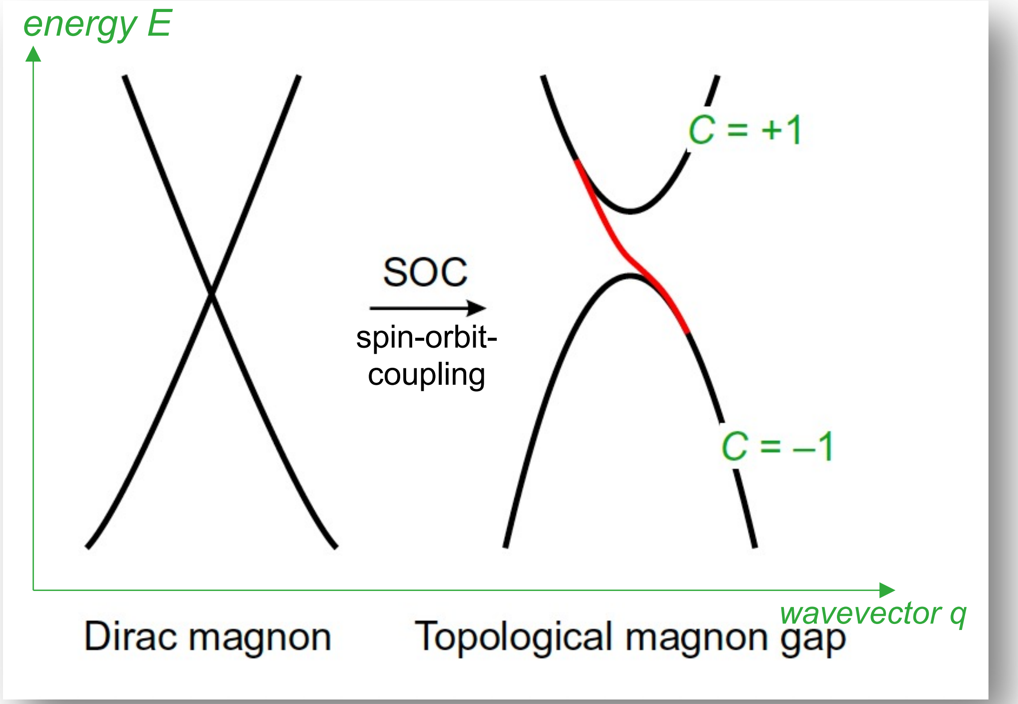
2D VAN-DER-WAALS HONEYCOMB FERROMAGNETS

Are $CrSiTe_3$ & $CrGeTi_3$ topological magnon insulators?



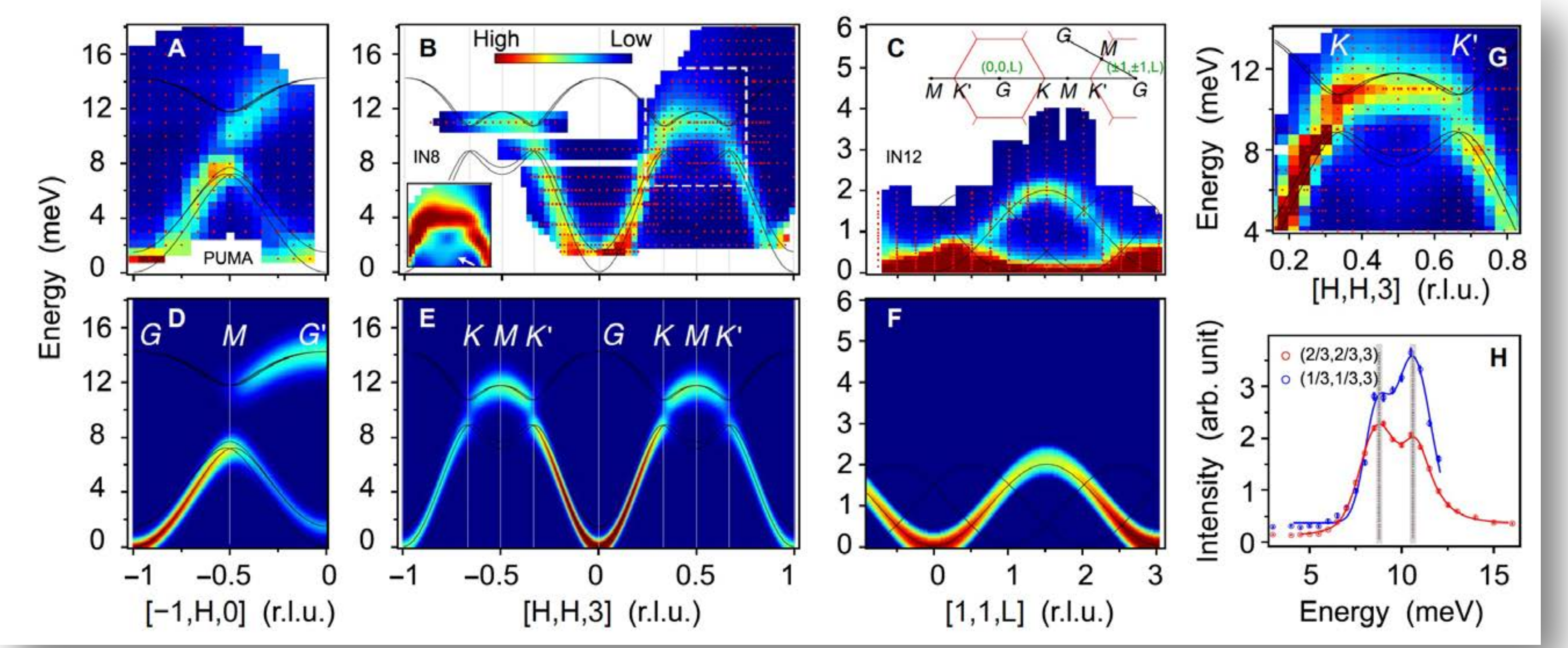




F. Zhu et al., Sci. Adv. 7 (2021) eabi7532

EVIDENCE FOR TOPOLOGICAL MAGNONS

Inelastic neutron scattering → Spin-wave excitations in $CrSiTe_3$



nontrivial gap at the K-point:

2 meV for $CrSiTe_3$

5 meV for $CrGeTe_3$

due to larger SOC

inelastic neutron scattering + theoretical analysis:

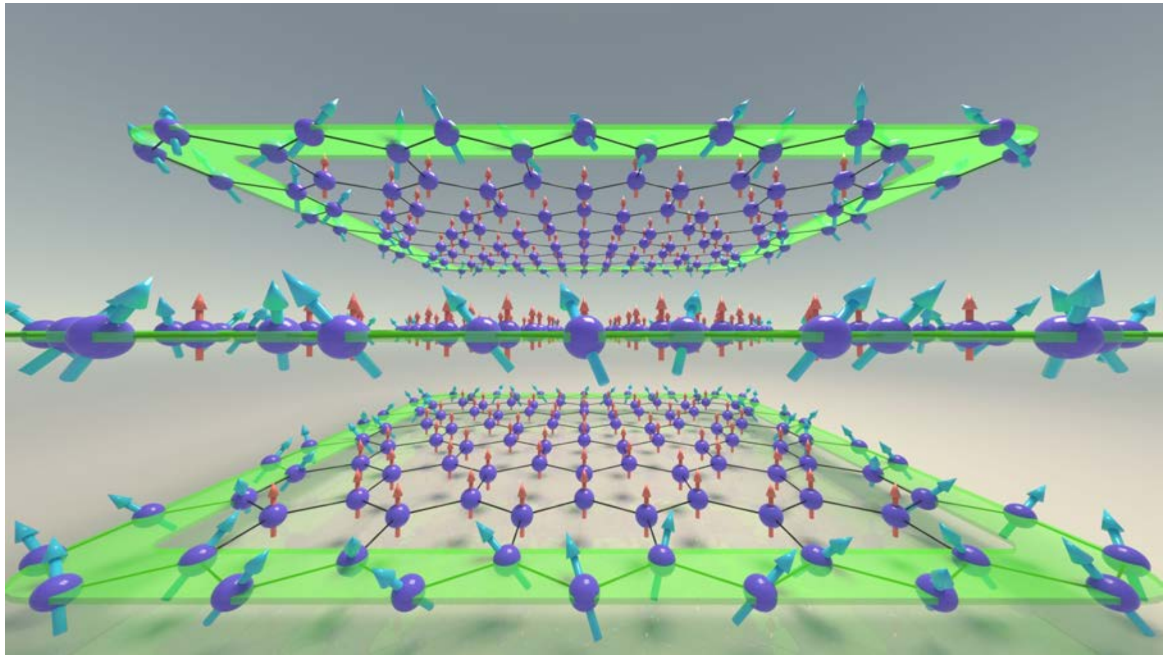
- nontrivial topological nature of the magnon band gap at the K points
- existence of topological edge states at the sample boundaries
- robust against disorder
- tunable gap through SOC of non-magnetic atom

F. Zhu et al., Sci. Adv. 7 (2021) eabi7532

TOPOLOGICAL MAGNON EDGE STATES

Towards energy efficient, fast and small IT devices

- nontrivial topology in a bosonic system realized (magnonic excitations)
- Such topological excitations and the corresponding nontrivial in-gap edge states are robust against disorder;
- the emergence and manipulation of the topological magnonic states bare a tremendous promise for future applications in magnonics and topological spintronics: energy efficient, fast and small IT devices



F. Zhu et al., Sci. Adv. 7 (2021) eabi7532

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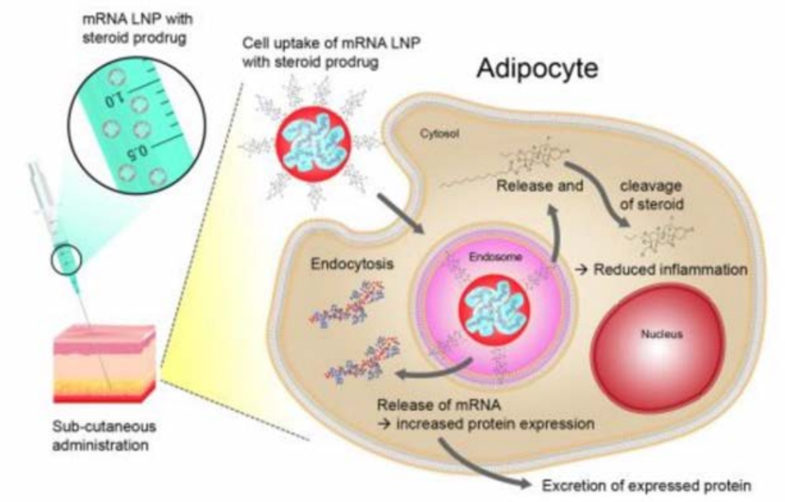
mRNA MEDICINES & mRNA VACCINES

Transfection: Lipid nanoparticles for transport into cells



Schematic representation of the administration of an mRNA treatment and the processes inside the cell. © AstraZeneca. First published in Nigel Davies et al.; Molecular Therapy: Nucleic Acid, Volume 24, 4 June 2021, Pages 369-384, DOI: 10.1016/j.omtn.2021.03.008 under Attribution-NonCommercial-NoDerivatives 4.0 International (CC BY-NC-ND 4.0)

AstraZeneca

Molecular Therapy 2021;
Proc. Natl. Acad. Sci. 2018

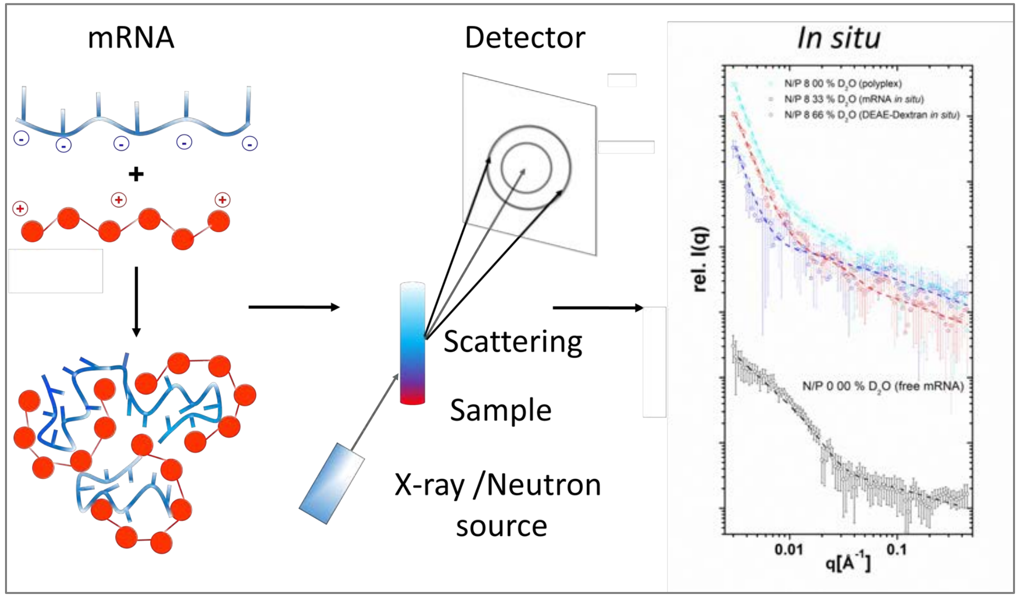
BIONTECH

Cells 2020, Biomaterials 2019
ACS Appl. Nano Mater. 2020

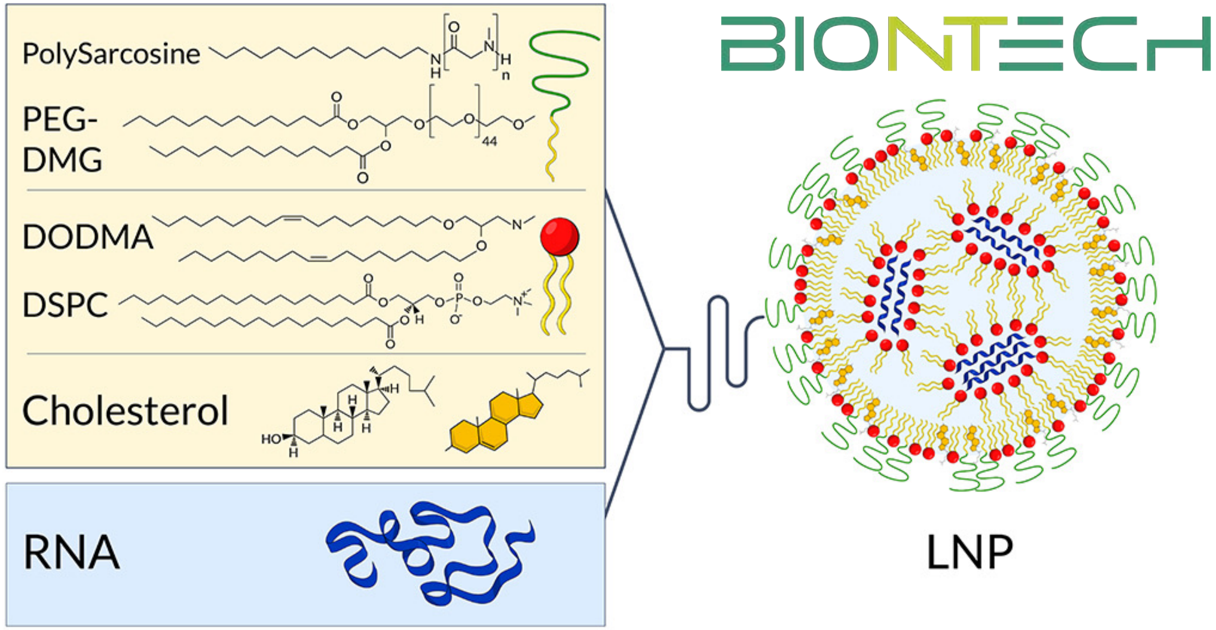
- mRNA: blueprint for production of protein molecules
- mRNA drugs could create proteins directly in the body,
- many potentially treatable diseases: cancer, haemophilia,…
- mRNA vaccines: well-known from covid
- how to introduce the mRNA into the cell?

NEUTRONS: REVEAL THE STRUCTURE BY SANS

with selective labeling through deuteration H → D



Results of the mRNA (in blue)/DEAE-dextran (in red) particles measured on the KWS-2 instrument (individual components and fully “visible” particles).

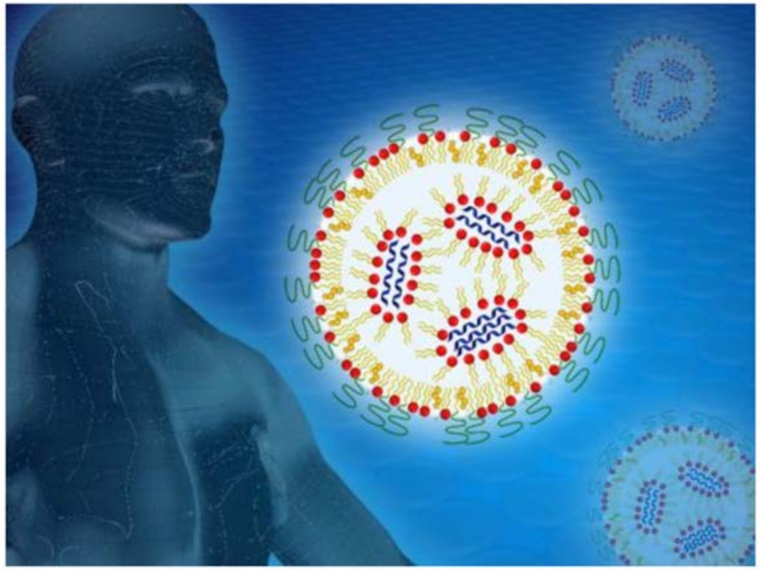


Schematic representation of a lipid nanoparticle with mRNA (blue).

D. Siewert et al., Cells 9 (2020), 2034 & Biomaterials, 2019
S S. Nogueira et al., ACS Appl. Nano Mater. 3 (2020), 10634–10645

OPTIMIZATION OF mRNA CONTAINING NANOPARTICLES

→ simplified method for the creation of mRNA nanoparticles with improved activity



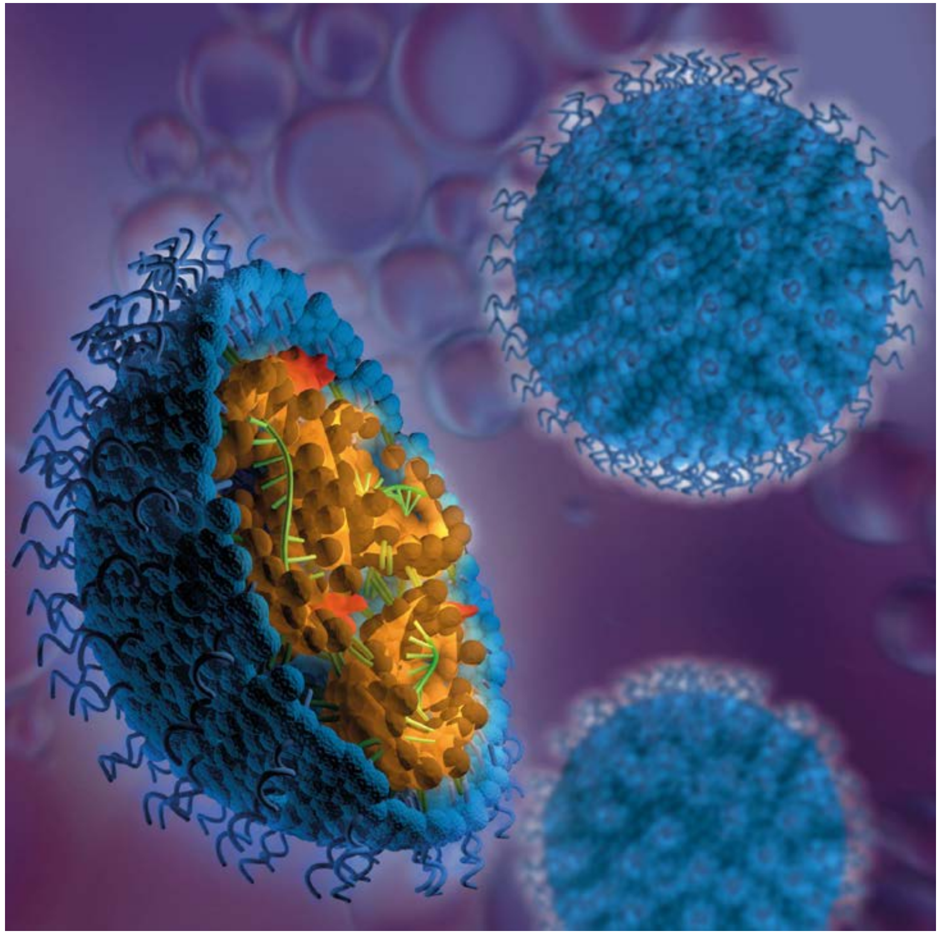
The spiral-shaped mRNA is packed in a lipid nanoparticle. The researchers made the individual structural components of the particle visible with the help of neutrons at FRM II.
© BioNTech / Reiner Müller, FRM

BIONTECH

Cells, 2020;
Biomaterials, 2019

AstraZeneca

Molecular Therapy 2021;
Proc. Natl. Acad. Sci. 2018



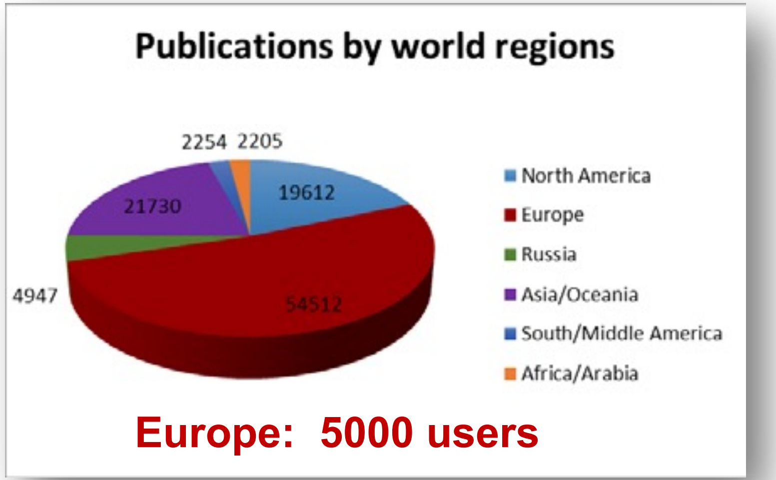
D. Siewert et al., Cells 9 (2020), 2034 & Biomaterials, 2019
S S. Nogueira et al., ACS Appl. Nano Mater. 3 (2020), 10634–10645

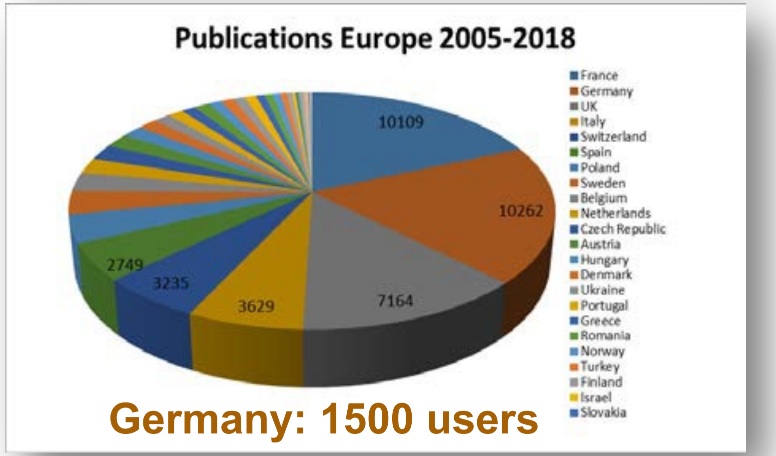
OUTLINE

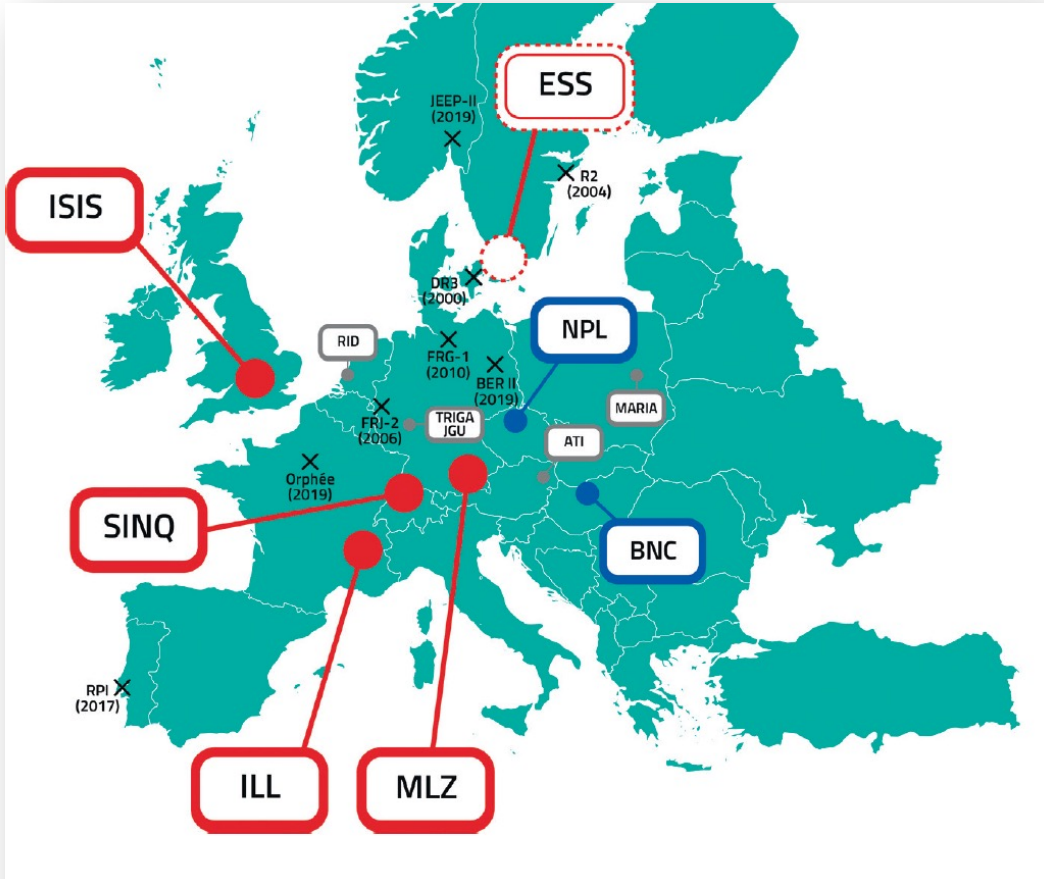
- Grand Challenge: Climate Crisis & Energy Transition
- Neutrons: Essential Tool for Energy Research – Batteries
- Neutrons: Essential Tool for Energy Research – Cooling
- Neutrons: Essential Tool for Energy Research & Information Technologies
- Neutrons: Essential Tool for Health Research
- **A New Tool for Research with Neutrons: The Next Generation Neutron Research Facility**
- Summary

EUROPEAN ECOSYSTEM 2030+: VULNERABLE!

Few major facilities for a leading community of 5000 users → vulnerable, capacity limited



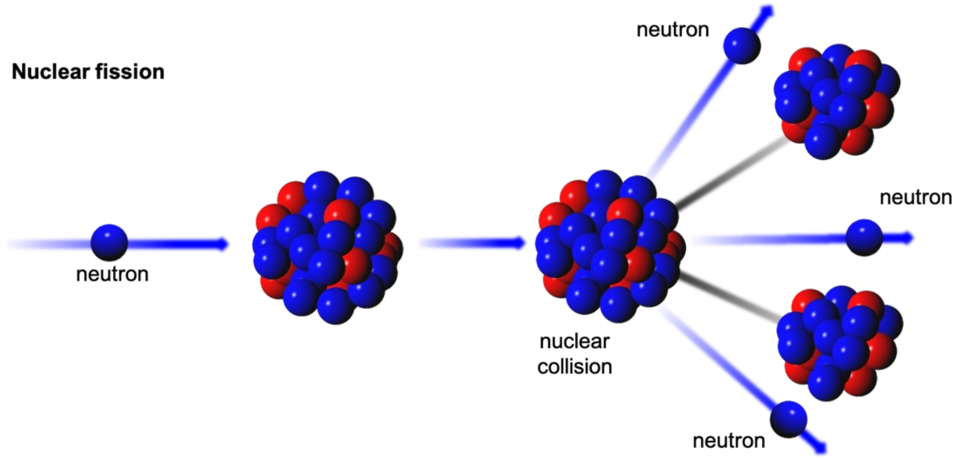


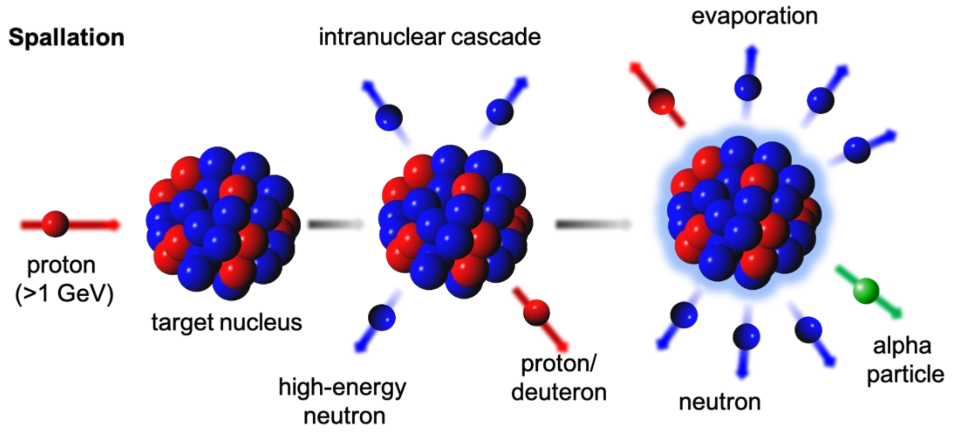


Neutron facilities in Europe. Larger facilities shown in red. Dashed lines indicate a facility that is under construction. Facilities that are no longer operating are marked with an x. © LENS - Stephanie Chapman

EUROPEAN NEUTRON ECOSYSTEM

Neutron production



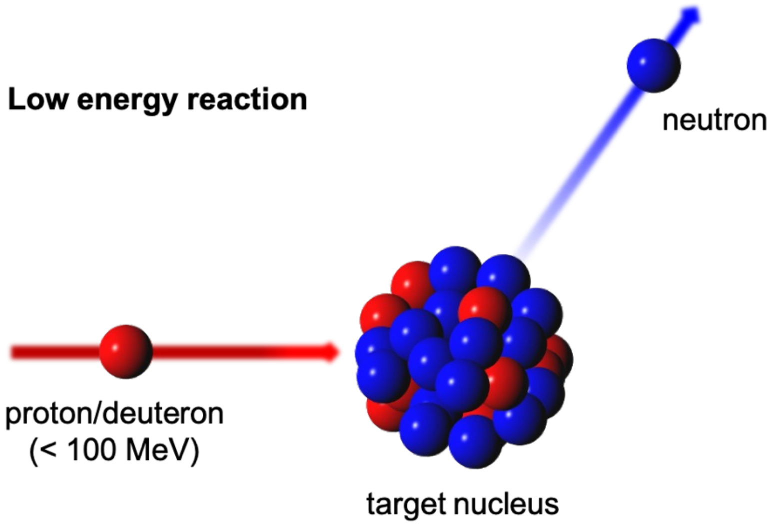


- **Fission**: existing research reactors reach end of their lifetime, except FRM II at Heinz Maier-Leibnitz Zentrum MLZ. New fission-based sources are not planned

- **Spallation**: two existing sources: ISIS (short pulse), SINQ (continuous). One under construction: ESS. New spallation sources have a high price tag (> 1 Billion Euro)

EUROPEAN NEUTRON ECOSYSTEM

CANS: at present only viable path towards the future ecosystem



- **CANS**: Compact Accelerator-driven Neutron Sources as local sources for specialized applications

- **HiCANS**: High Current Accelerator-driven Neutron Sources as a novel approach to produce high brightness neutron beams for highly competitive instruments; have the potential to replace the ageing fission-based sources as user facilities

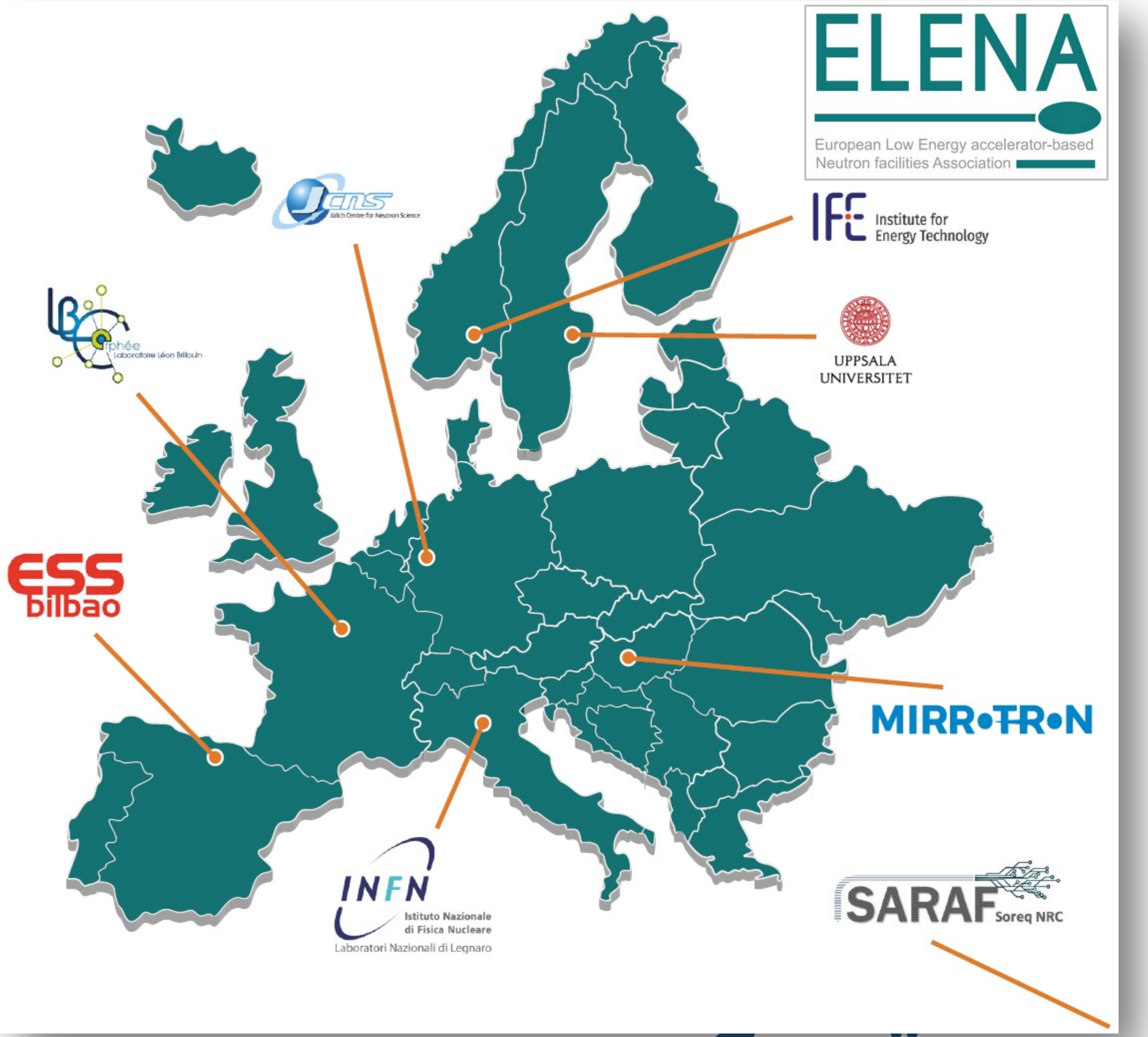
CANS & HiCANS FOR A SUSTAINABLE ECOSYSTEM!

Projects within the European Low Energy accelerator-based Neutron facilities Association (ELENA)

LENS LEAGUE OF ADVANCED EUROPEAN NEUTRON SOURCES

"Neutron Science in Europe"

- Though ESS will provide enhanced capabilities, these can only be fully exploited if the supporting ecosystem has sufficient strength, depth and diversity.
- The only route for entirely new facilities with significant capacity are High Current Accelerator-driven Neutron Sources …



COMPETITIVE INSTRUMENTS BY FACILITY DESIGN

HBS: A High Current Accelerator-driven Neutron Source (HiCANS)

high current accelerator → HiCANS

- 100 mA, 70 MeV for increased source strength
- adapted macro bunch filling pattern

several target stations

- deserved by multiplexer
- optimized pulse structure (length, frequency)

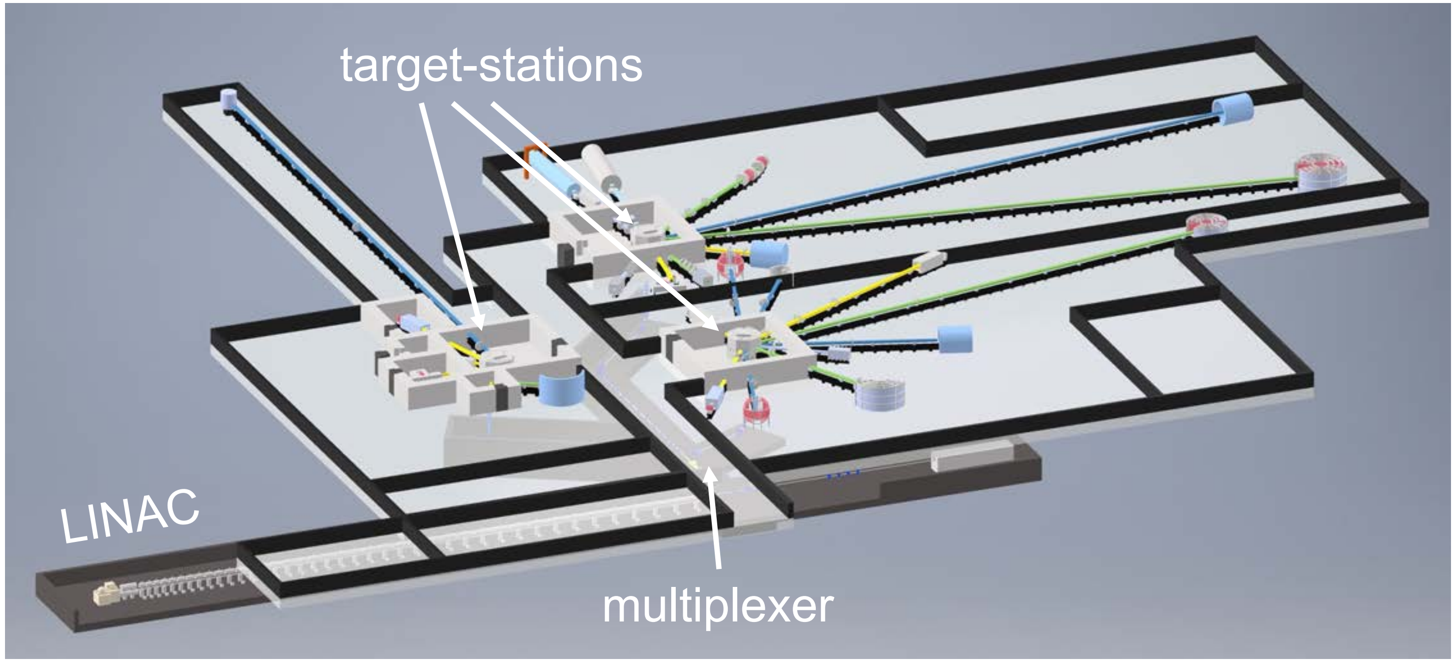
every beam port serves 1 instrument

- optimized source spectrum and geometry
- neutron optics integrated in beam port

compact shielding → neutron optics

- optical elements positioned close to moderator
- optimal phase space extraction

Facility layout with 3 target stations
and a reference suite of 25 instruments



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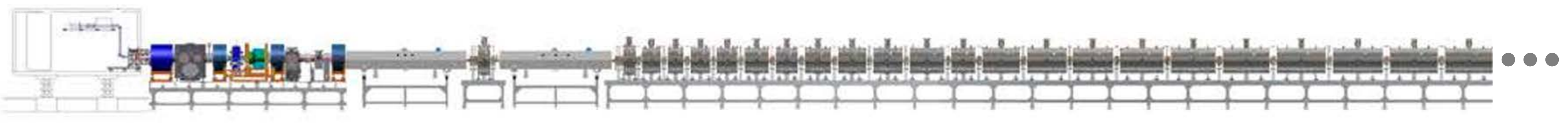
HIGH CURRENT LINAC: RISK MINIMIZATION, RELIABILITY

Efficient, flexible, reliable, conservative

low energy & high beam power & low-to-medium duty cycle → room temperature operation
eliminates need for cryogenic facility and allows **recourse to technology developed for the MYRRHA project**



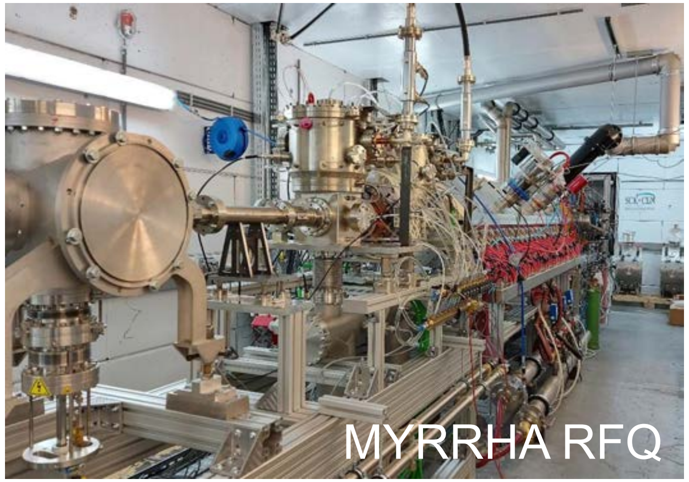
ECR source *LEBT* *RFQ /MEBT/ RFQ* *CH-DTL*

> 120 mA *ExB-Ch.* *→1.2 MeV→2.5 MeV* *→→ 70 MeV, 100 mA, 4.8% beam duty, 96/96/24 Hz*

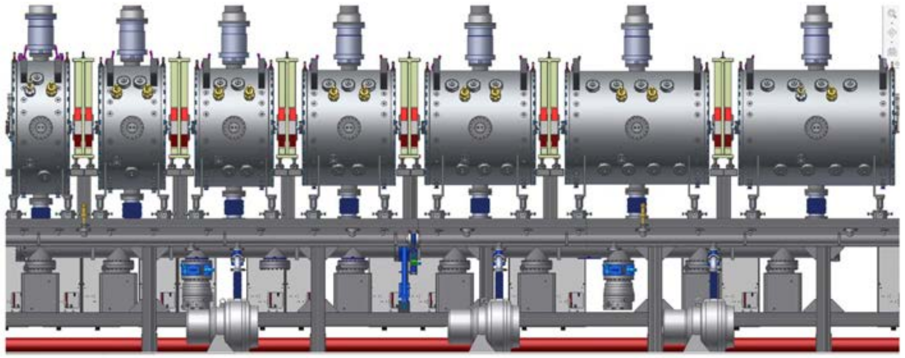
GOETHE UNIVERSITÄT FRANKFURT AM MAIN

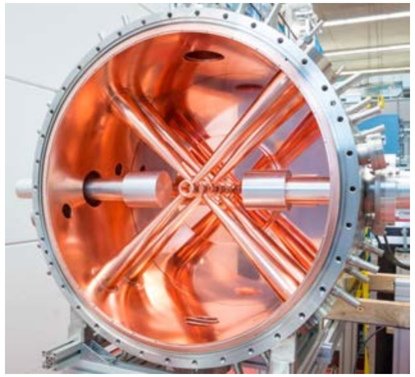
iAP Institut für Angewandte Physik

HOLGER PODLECH



MYRRHA RFQ





CH-DTL

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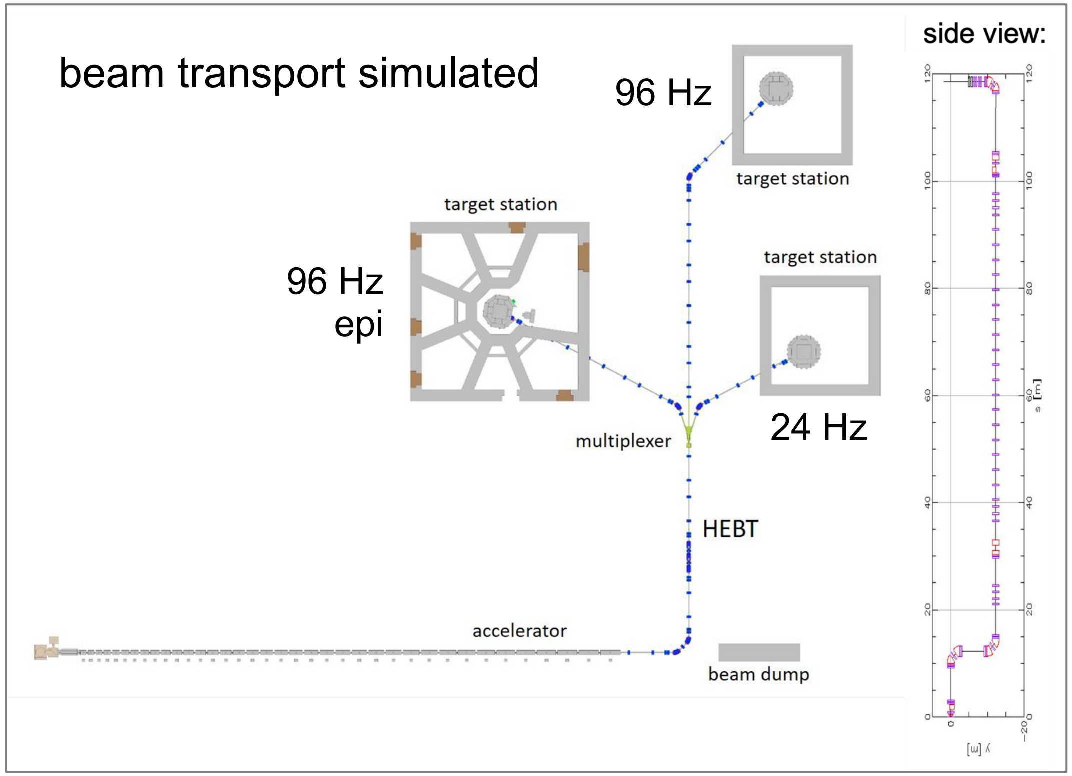
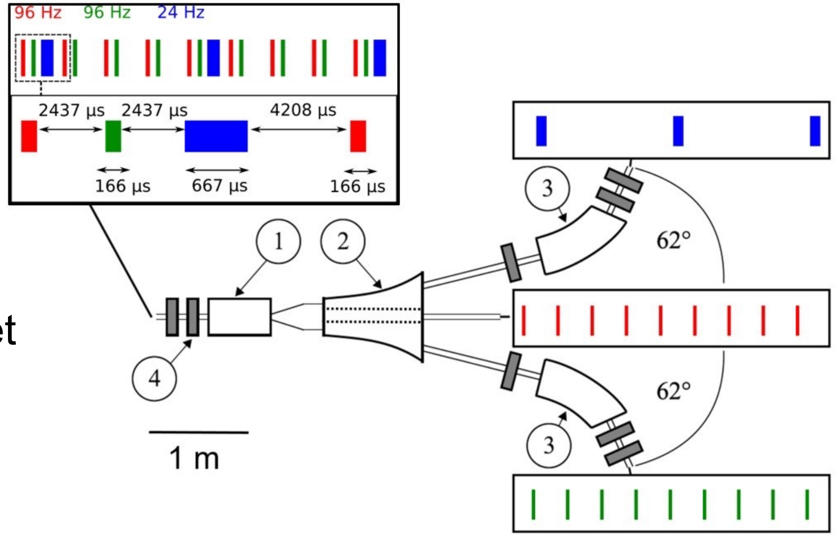
DESERVING SEVERAL TARGET STATIONS

High Energy Beam Transport (HEBT) simulated and multiplexer (prototype exists)

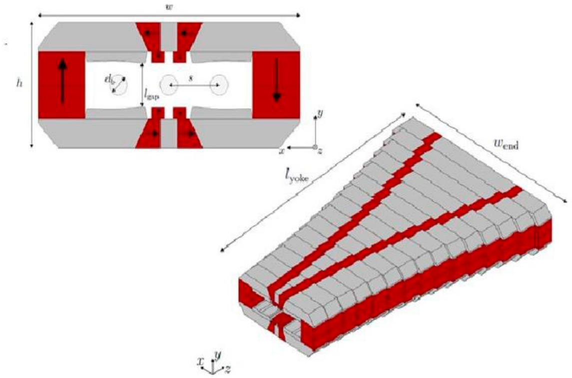
high energy beam transport (HEBT):



multiplexer:



1: kicker magnet
2: septum magnet
3: dipoles
4: quadrupoles



newly developed three-field septum magnet:
prototype tested ✓

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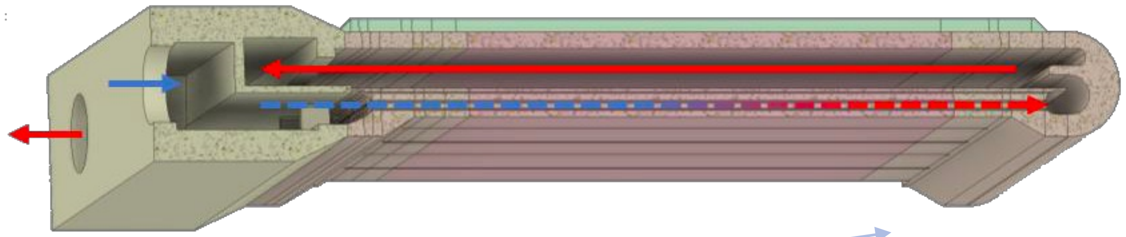
HIGH POWER TARGET: SUCCESSFULLY TESTED!

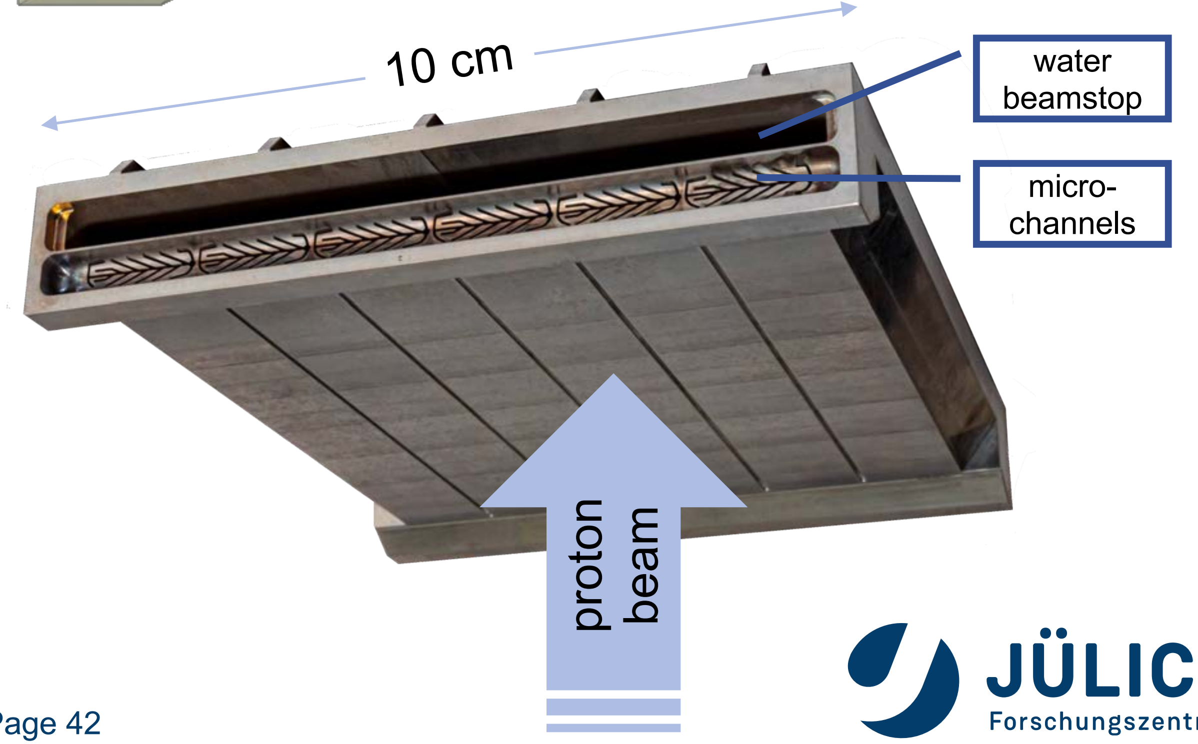
Newly designed high-power target with long lifetime for high source strength

design criteria: 70 MeV proton beam of 100 kW power on 100 cm^2 target area for a lifetime of one year (5000 h) and maximum source strength

Tantalum target for
- ✓ high neutron yield
- ✓ high hydrogen solubility
- ✓ high yield strength
- ✓ low embrittlement in radiation field
- ✓ good thermal conductivity
- ✓ high melting point
- ✓ good mechanical workability
- ✓ chemically inert and erosion resistant
- ✓ low activation

Fishbone microchannel structure **tested for**
- ✓ **heat load (1 kW/cm^2)** with e-beam facility
- ✓ **water erosion:** endurance flow test

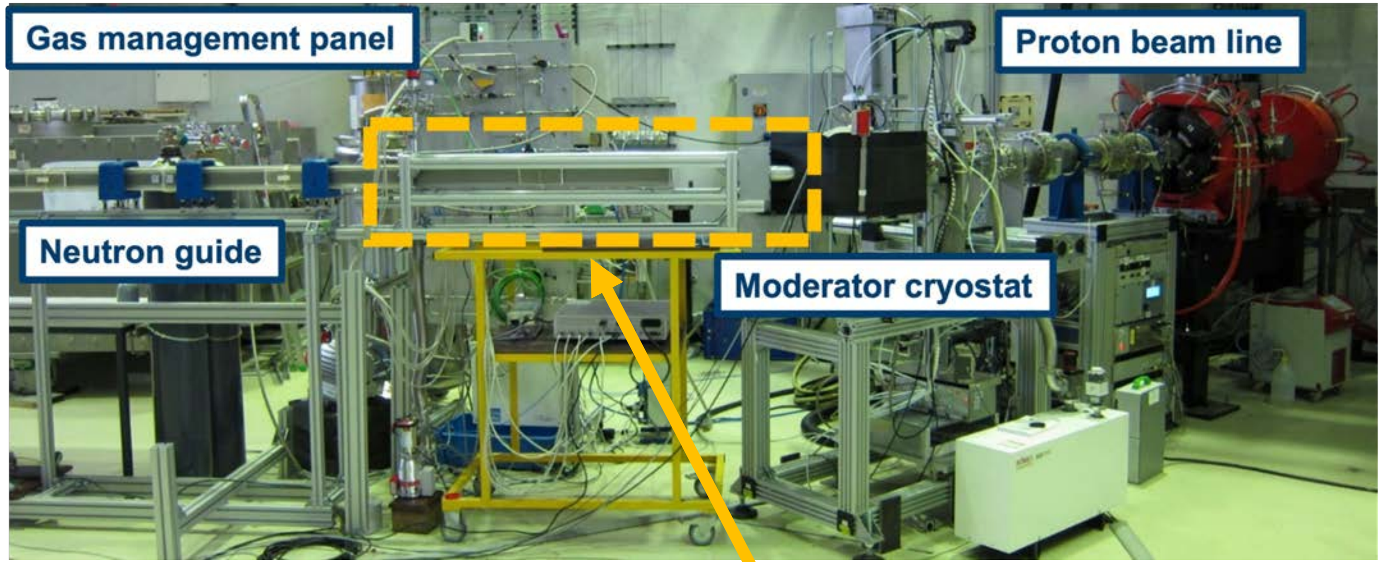


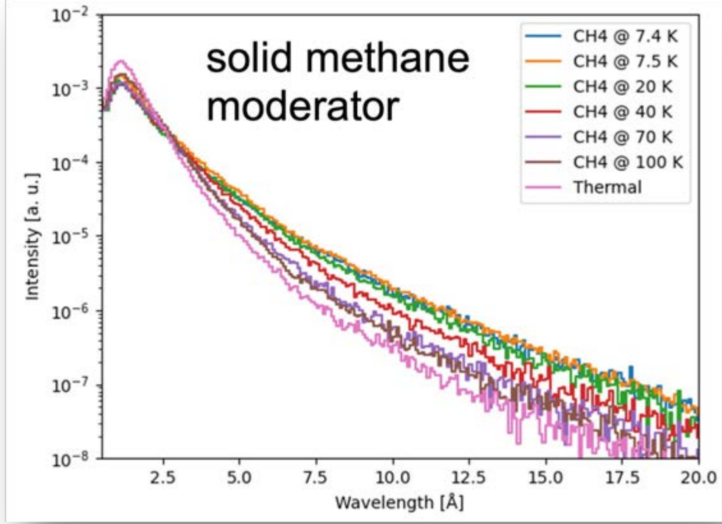


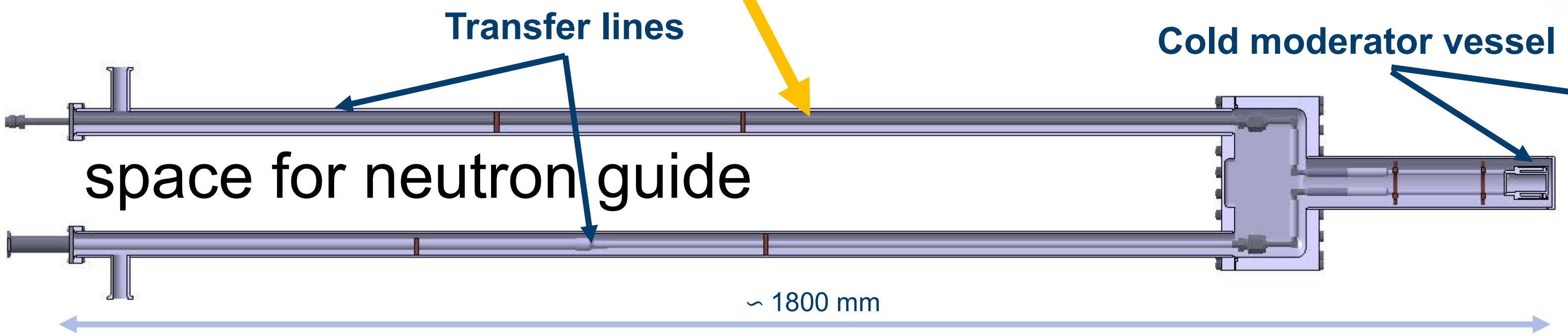
FINGER MODERATOR: FIRST REALIZATION & TEST

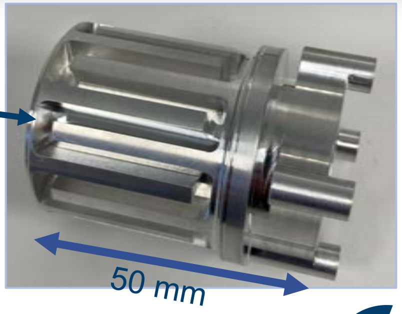
Time-of-flight measurement at BigKarl facility with 40MeV 10 μA proton beam

✓ **4 types of cold moderators tested:**
- solid mesitylene C_9H_{12}
- liquid hydrogen H_2
- solid methane CH_4
- liquid para-hydrogen p-H_2 (first ever!)









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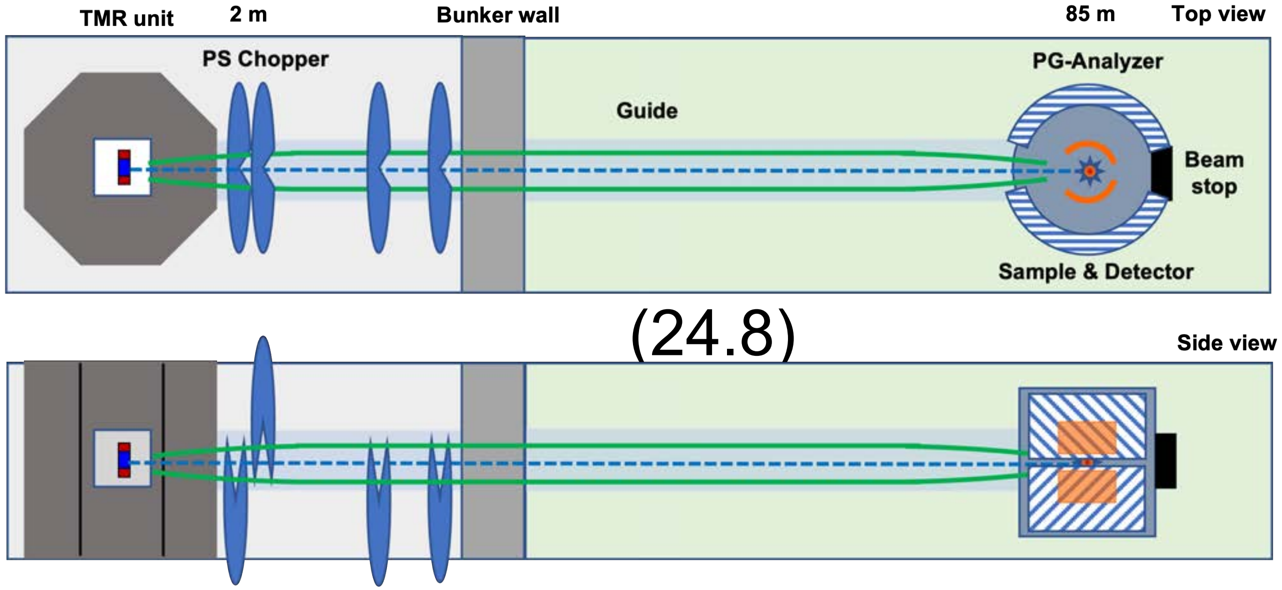
EXAMPLE: NEAR BACKSCATTERING SPECTROMETER

Optimal phase space extraction & prismatic focusing → very high intensities!

separation of coherent and incoherent scattering and background reduction with polarized neutrons
energy material systems, dynamics in life sciences



- 24 Hz target station
- primary flight path 85m
- $\delta\lambda/\lambda \geq 5 \cdot 10^{-4}$
- 5 μeV energy resolution

✓ **flux comparable to BASIS @ SNS**:
(24.8): $8 \cdot 10^6$ n/cm^{2}s simulated,
within ≈ factor 2 of BASIS

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HBS: THE NEXT-GENERATION NEUTRON FACILITY

A national neutron facility for science and industry with unique selling points

breaking with seemingly well-established certainties → based on fresh thinking!

a highly efficient neutron facility	offers cost-efficient neutron provision for highly competitive instruments *low energy accelerator, small target, compact shielding*
changes the paradigm of neutron facilities	the source becomes integral part of the instrument *with optimized pulse structure, spectrum & beam extraction*
sustainable & accessible	minimizes radioactive waste and requires no nuclear licensing *easy access for users from science and industry*
opportunities for innovation and technology	novel technologies and attractive access schemes *innovation during construction and operation*
resilient & flexible	modular design, can be adapted to specific requirements *minimizes down times, flexible set-ups*

TDR IN 4 VOLUMES PLUS SUMMARY

Technical Design Report (TDR) nearly finished

TDR Accelerator

Executive editors:

H. Podlech (IAP Frankfurt)
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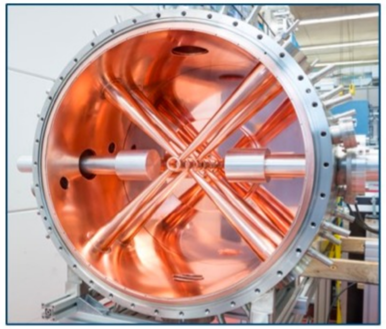
R. Gebel (IKP-4)



100 %

TDR Neutron Target

Executive editors:

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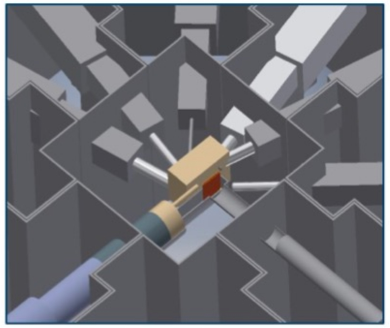

85%

TDR Neutron Instruments

Executive editors:

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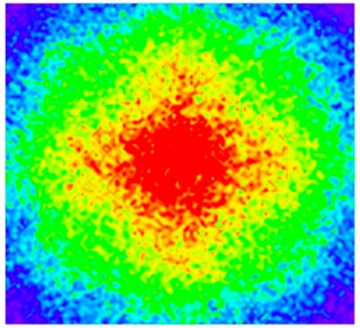

100 %

Infrastructure & Sustainability

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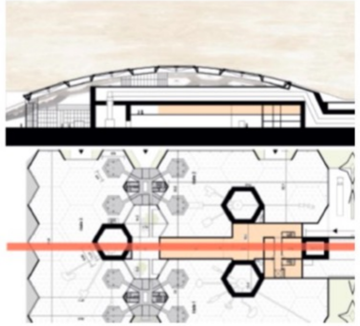
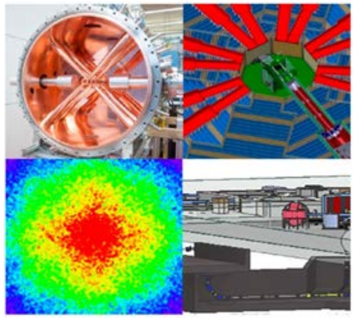


70%



Technical Design Report HBS
Preliminary Summary

T. Brückel, T. Gutberlet (Eds.)

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(percentage of completion)

✓ TEST-FACILITY AT FZJ COMMISSIONED

First beam on target on Dec. 12, 2022, with 3 beamlines in operation

proton beamline from cyclotron

- 45 MeV pulsed protons, only nano Ampere current

target-moderator-reflector (TMR) unit

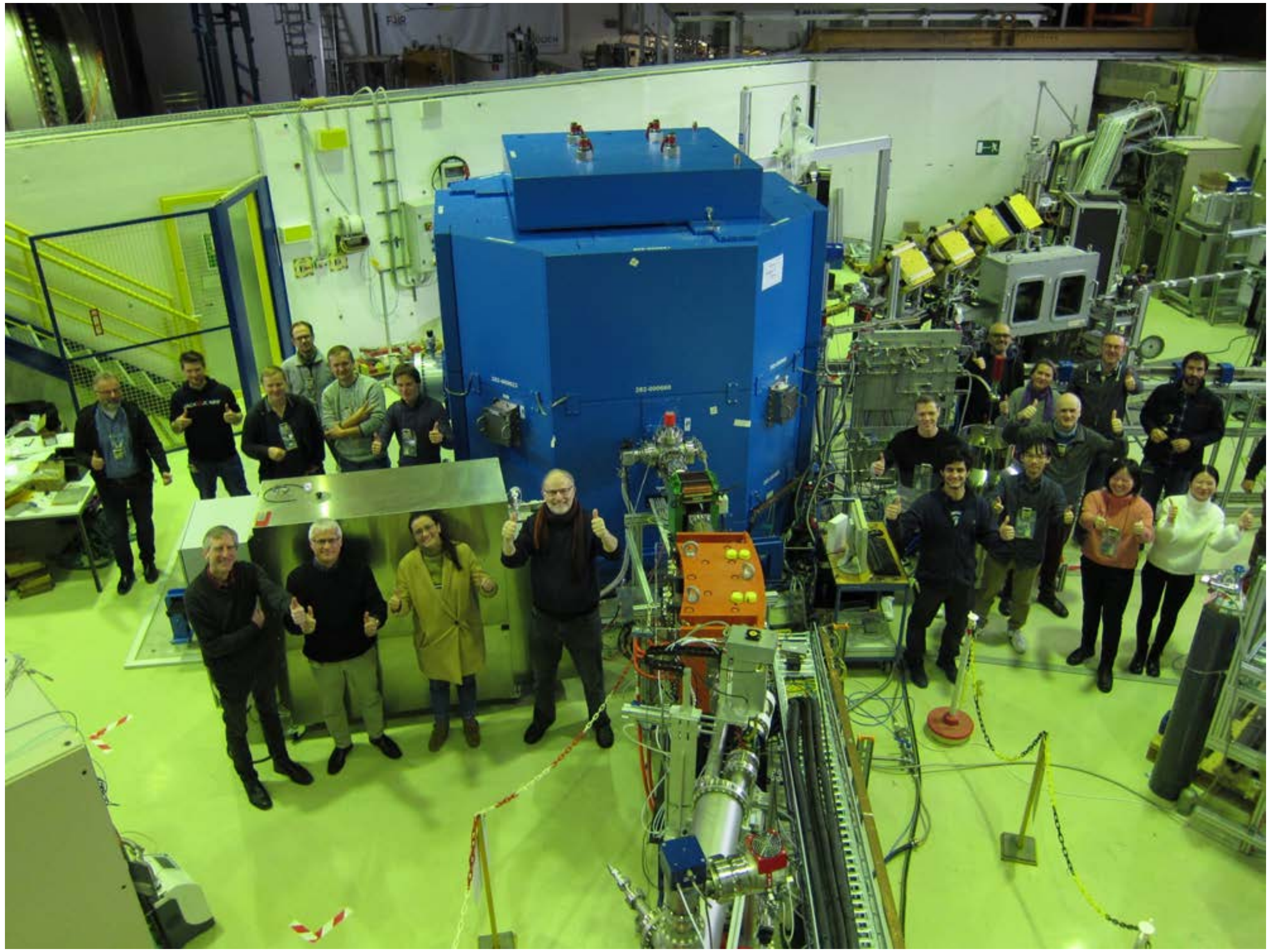
- HBS Ta-target, PE-moderator, Pb-reflector

cold methane moderator

- spectrum measured at various temperatures

three beamlines in operation

- time-of-flight diffractometer: neutron energy spectrum, first diffractogram
- HERMES reflectometer provided by LLB: total reflection edge of supermirror
- detector test station: SONDE detector for ESS tested



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/ HIM
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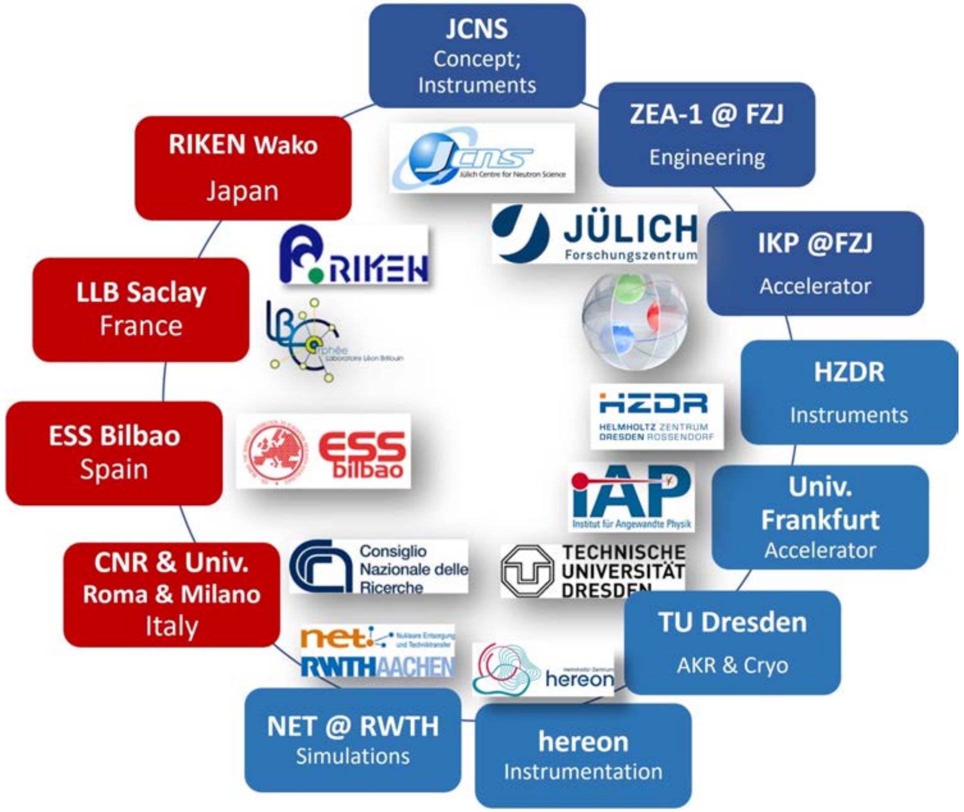
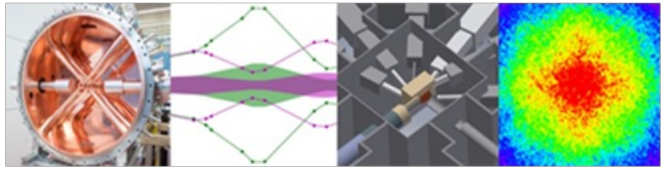
J. Fenske

- Instrumentation



HBS Innovationpool Project



FB Matter: MML, MT

Federal Ministry of Education and Research

Th. Stöhlker

FROM MATTER TO MATERIALS AND LIFE

European Low Energy accelerator-based Neutron facilities Association

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