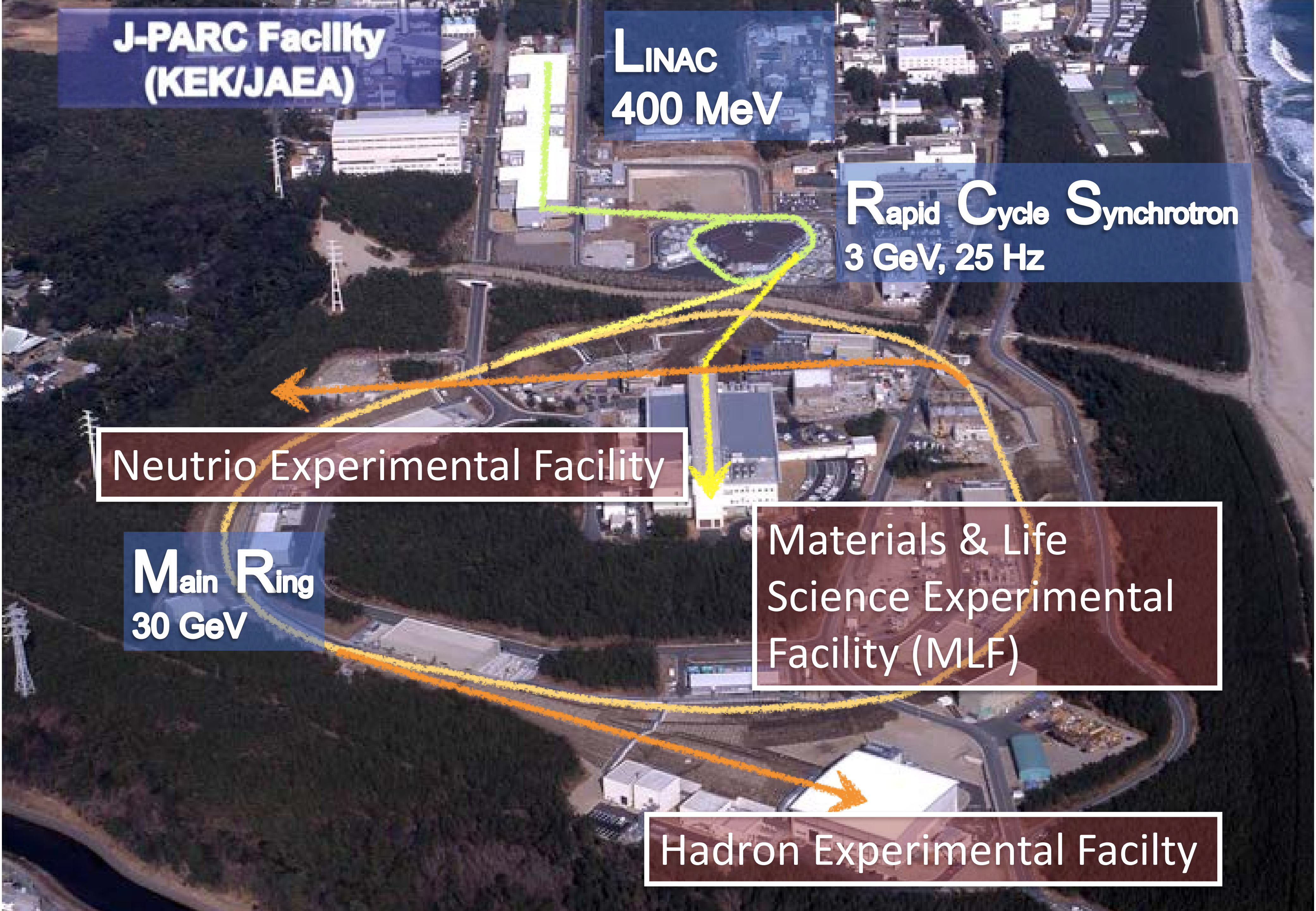
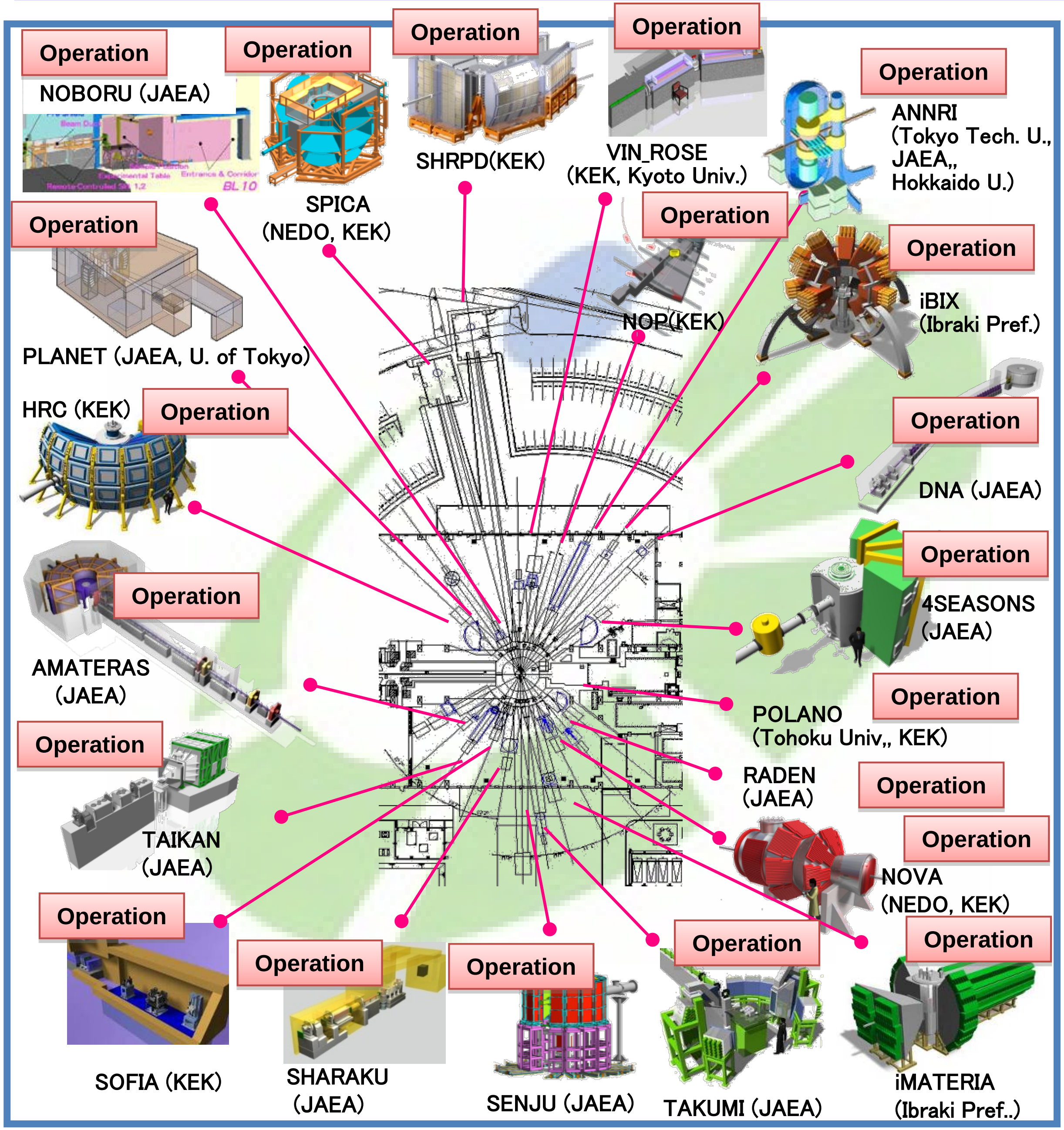
Element Strategy Initiative Advisory Council 2019
December 13, 14, 2019

Particle beam facility
J-PARC MLF

Toshiji Kanaya
J-PARC MLF

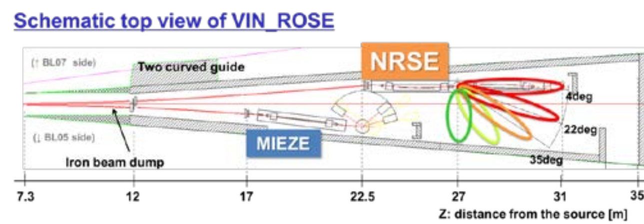

J-PARC Facility
(KEK/JAEA)
LINAC
400 MeV
Rapid Cycle Synchrotron
3 GeV, 25 Hz
Neutrio Experimental Facility
Main Ring
30 GeV
Materials & Life
Science Experimental
Facility (MLF)
Hadron Experimental Facilty

Neutron Instruments at MLF



- 23 Neutron Beam Ports
- Operation: 21 (April, 2019)

VIN-ROSE (NSE): opened to users @2017B



POLANO
(Polarization Analysis Spect.)

Opened to users @2019A

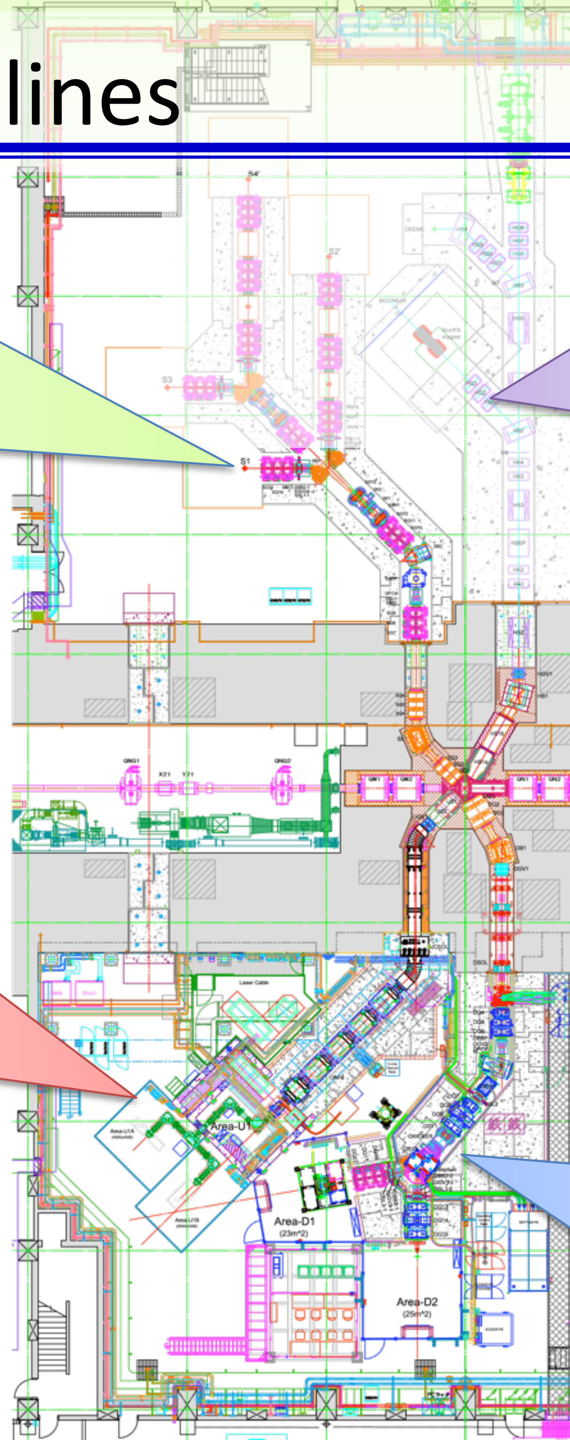
4 Muon beam lines

S-line μ^+

Slow beam (4 MeV), dedicated to bulk μSR ultralow temperature/high magnetic field/pulsed excitations.
(S1:2016~)

U-line μ^+

Ultra slow beam (0.1 ∼ 30 keV), near-surface, sub-micron scale condensed matter physics, chemistry, etc.



H-line $\mu^\pm$

Slow (4 MeV) ∼ fast (50 MeV) beam, for particle physics, atomic physics ("precision frontier")

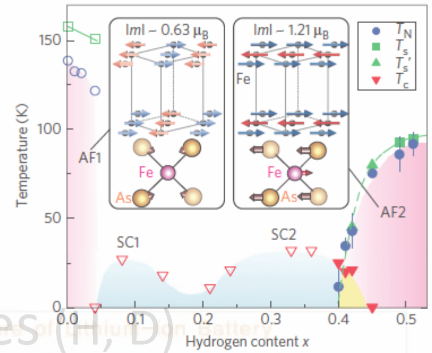
D-line $\mu^\pm$

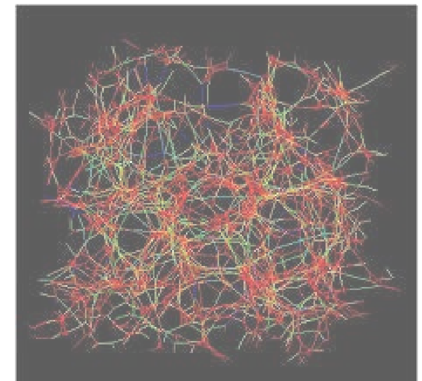
Slow (4 MeV) ∼ fast (50 MeV), general-purpose beamline with 2 exp. areas.
(2009~)

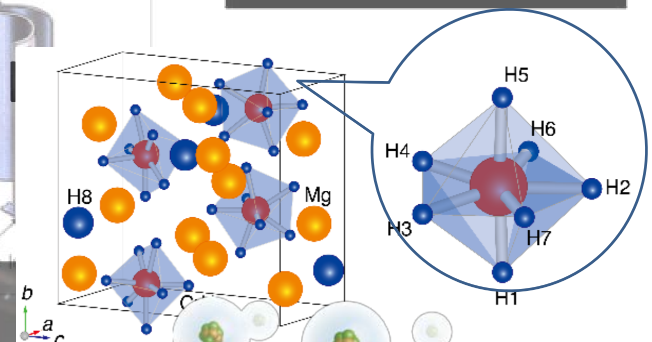
Focusing Science Areas in MLF

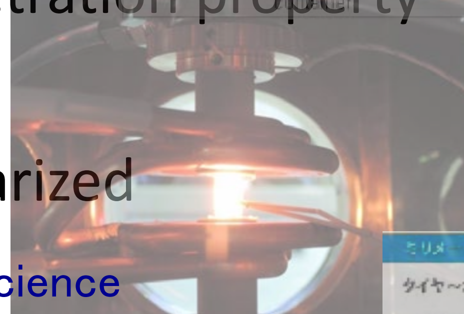
Based on characteristic features of neutron and muon

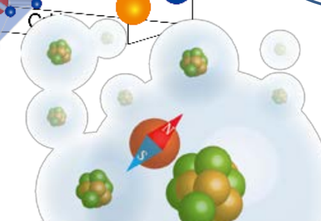
- Hard Matter
  - Neutron has spin=1/2
- Liquid and Soft Matter
  - Neutron can distinguish isotopes (H, D)
- Energy Material
  - Neutron is sensitive to light elements (H, L
- Engineering Material
  - Neutron has deep penetration property
- Muon Science
  - Muon is inherently polarized

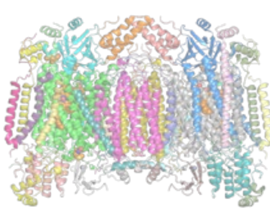












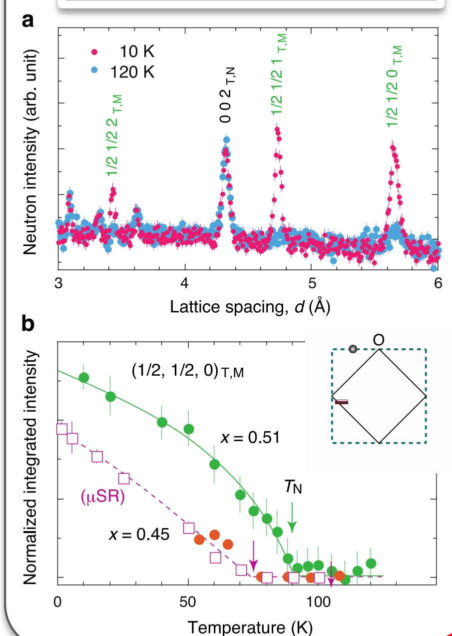
Life Science
High pressure science
Industrial Application

Fe-based superconducting material $LaFeAsO_{1-x}H_x$ using multi-probe analysis

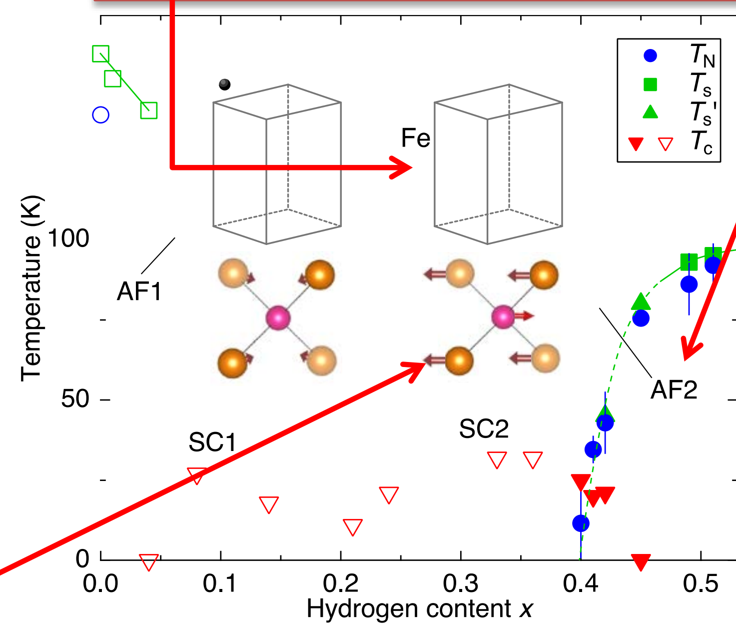
Professor H. Hosono
ITES, ITI

Discovery of a new magnetic phase (AF2) and its contrasting properties to the original one (AF1)

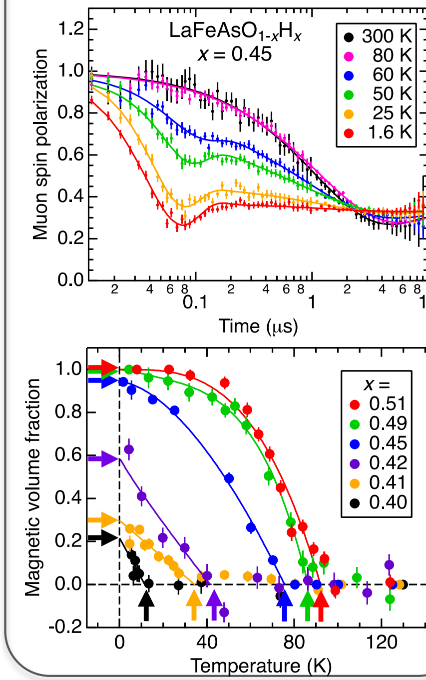
magnetic structure (neutron)



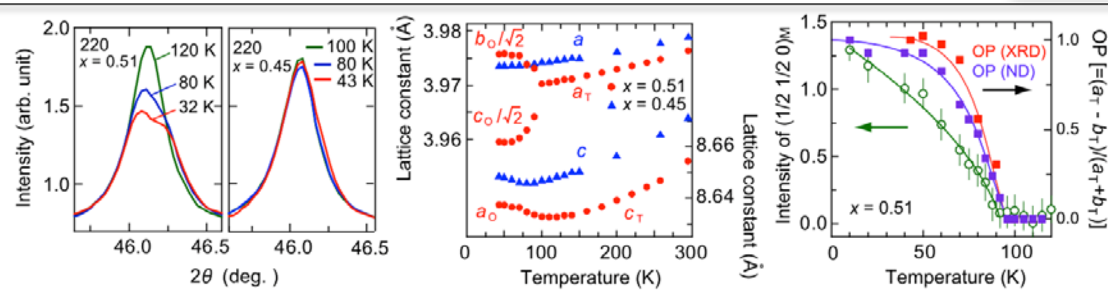
Structural and magnetic phase diagram of $LaFeAsO_{1-x}H_x$



magnetic phase diagram (muon)



Crystal structure (X-ray)



Nature Physics 10, 300 (2014).

Role of Hydrogen in Electronic Materials Inferred by Muon

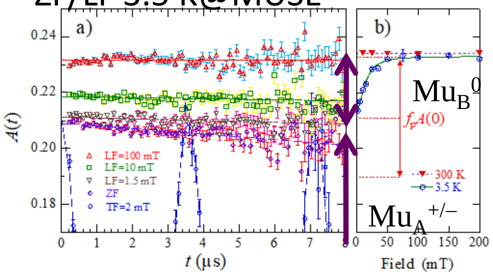
Muon = Pseudo-hydrogen

FeS_2 (pyrite)

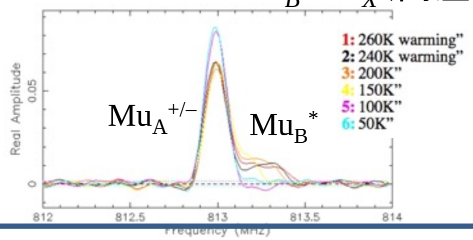
Issue: Is H electrically active in FeS_2 ?

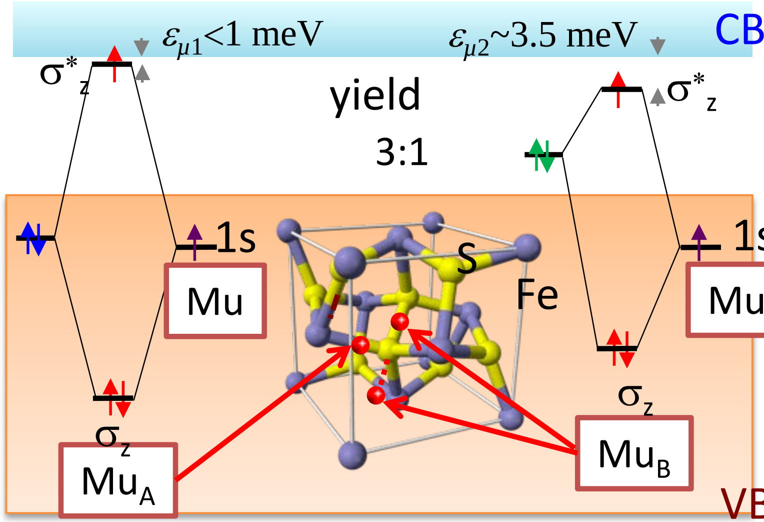
H. Okabe *et al.*, Phys. Rev. B **98**, 075210 (2018). [Featured by APS Blog]

ZF/LF 3.5 K@MUSE



TF=6 T@TRIUMF $k_B T > \varepsilon_X$（高温）





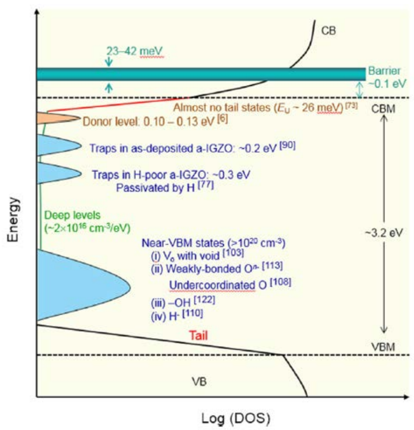
Mu+/S-S bond break → Radical-A＋SMu^-

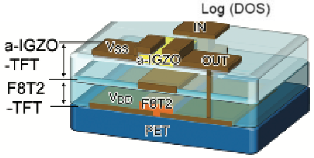
Mu+Fe-S bond break → Radical B＋SMu^-

Answer: Yes, two different Mu states bound to sulfur, serving as donors.

InGaZnO (IGZO)

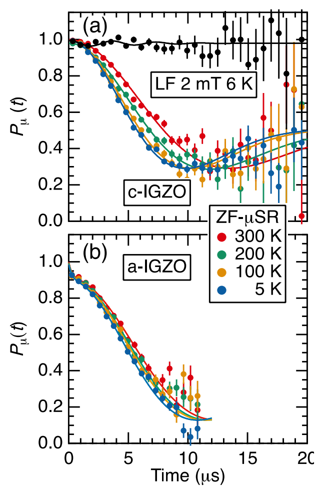
Issue: What is the role of H for the in-gap states of IGZO?

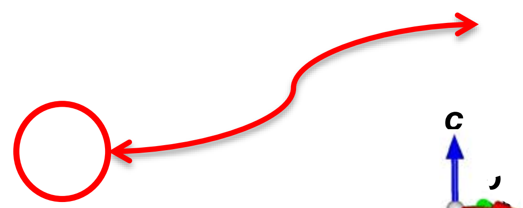




ZF/LF 3.5 K@MUSE

K. M. Kojima *et al.*, Appl. Phys. Lett. **115**, 122104 (2019).[Editors pick]





Answer: Shallow donor at ZnO bond center, or [H Mu]$^{2-}$ complex in O vacancy.

Mu site was estimated by nuclear dipolar field Δ and DFT calc.

Engineering Materials

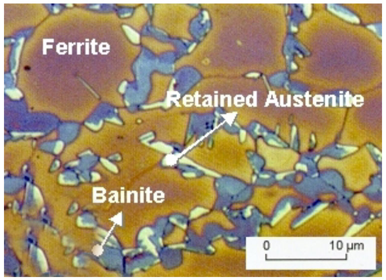
constructed in 1887 – 1889	1957 – 1958	2008 – 2012
height 324m	height 333m	height 634m
7300 t (wrought iron!)	4000 t (steel)	32000 t
160~220N/mm^2	240N/mm^2	400N/mm^2
0.05~0.25wt%C	0.3~2wt%C	700N/mm^2 (gain tower)
		Mn, Ni, Mo addition ~0.1%C

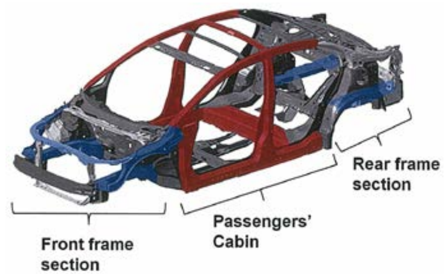
Steel is still developing in strength

Development of high performance steel (TRIP, TWIP...)
Strength and Ductility - microstructure control

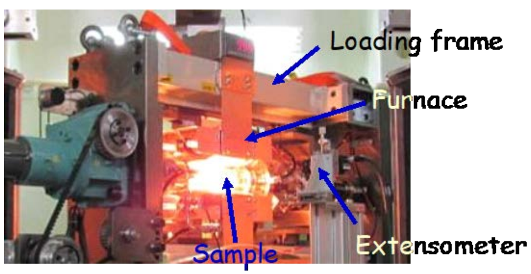
Professor T. Tanaka
(ESISM, Kyoto Univ.)

Control of crystal grain structure during the processing is a key to obtain the high performance.

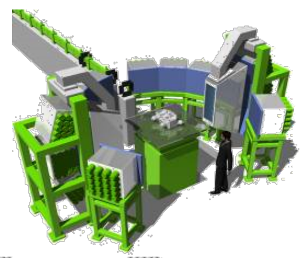


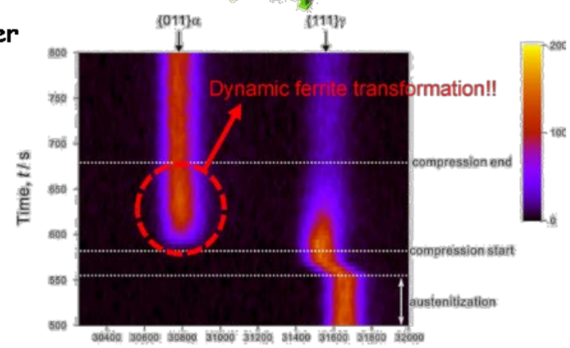


Thermo-Mechanical Processing Simulator (Thermec-Master) into TAKUMI (BL19)
(The Elements Strategy Initiative)



- High-frequency induction heating & servo motor driving
- Gas (N_2, He) injection cooling
- Highest temp: 1200 C
- Heating/cooling rate ≤ 30C/s
- Deformation rate ≤ 100 mm/s, 30 kN (compression)

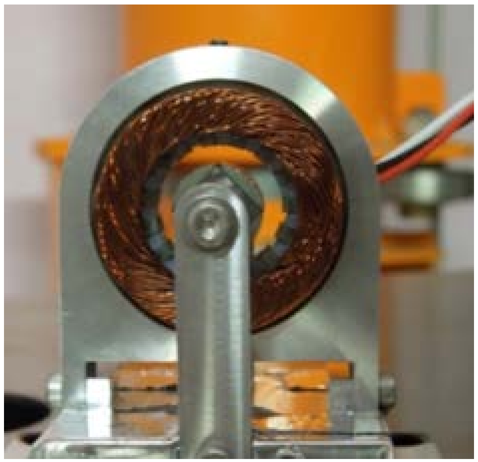


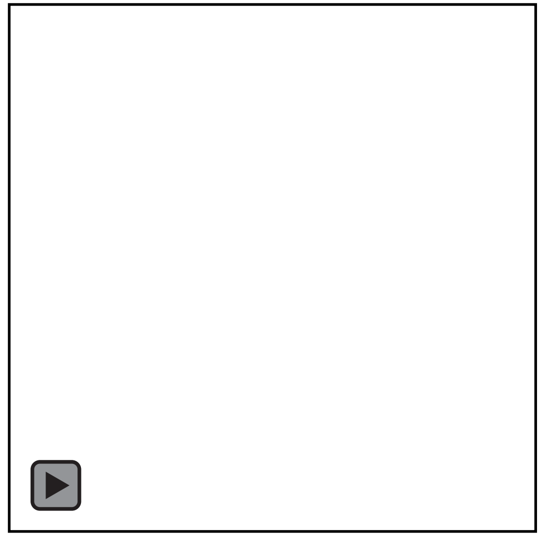


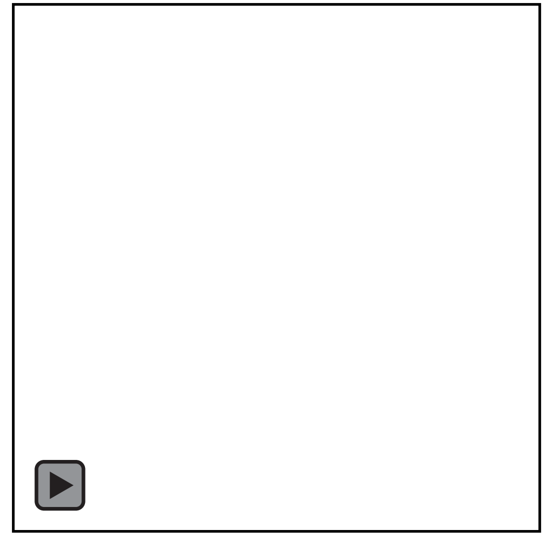
Ferrite transformation is accelerated by hot compression -> Dynamic transformation

Yoshihiko Nakamura *et al.*, submitted to Special Issue by The Mineral, Metals & Materials Soc.

Magnetic Imaging @ RADEN



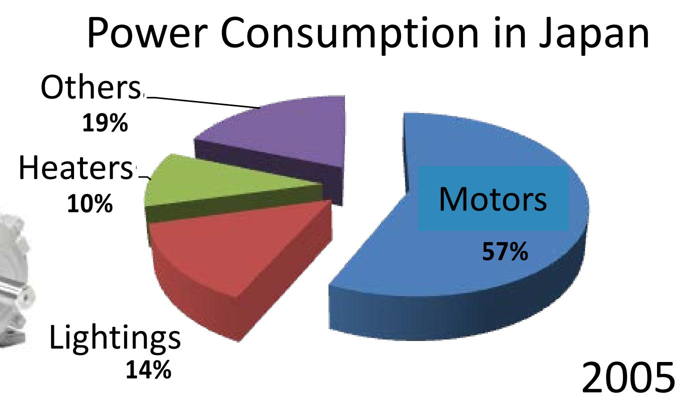




The world's 1st demonstration of visualizing magnetic field of a working motor.

Collaboration with Hitachi Ltd. HITACHI Inspire the Next

RADEN results are used to improve simulation technology to design higher performance motors.



Motors consume more than 50% of total electric power in Japan

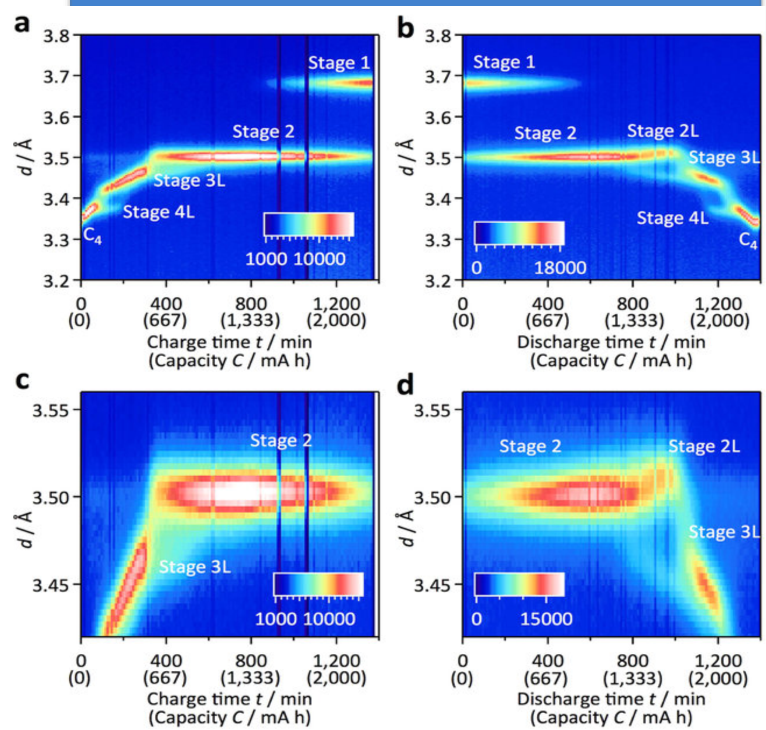
Supported by Photon and Quantum Basic Research Coordinated Development Program by MEXT (2013-2018)

Research & Development Initiative of New Generation Batteries

SPICA (BL09) is a dedicated machine to the project for battery research

Real-time observations of lithium battery reactions during the charging and discharging process
Scientific Reports **6**, Article number: 28843 (2016)

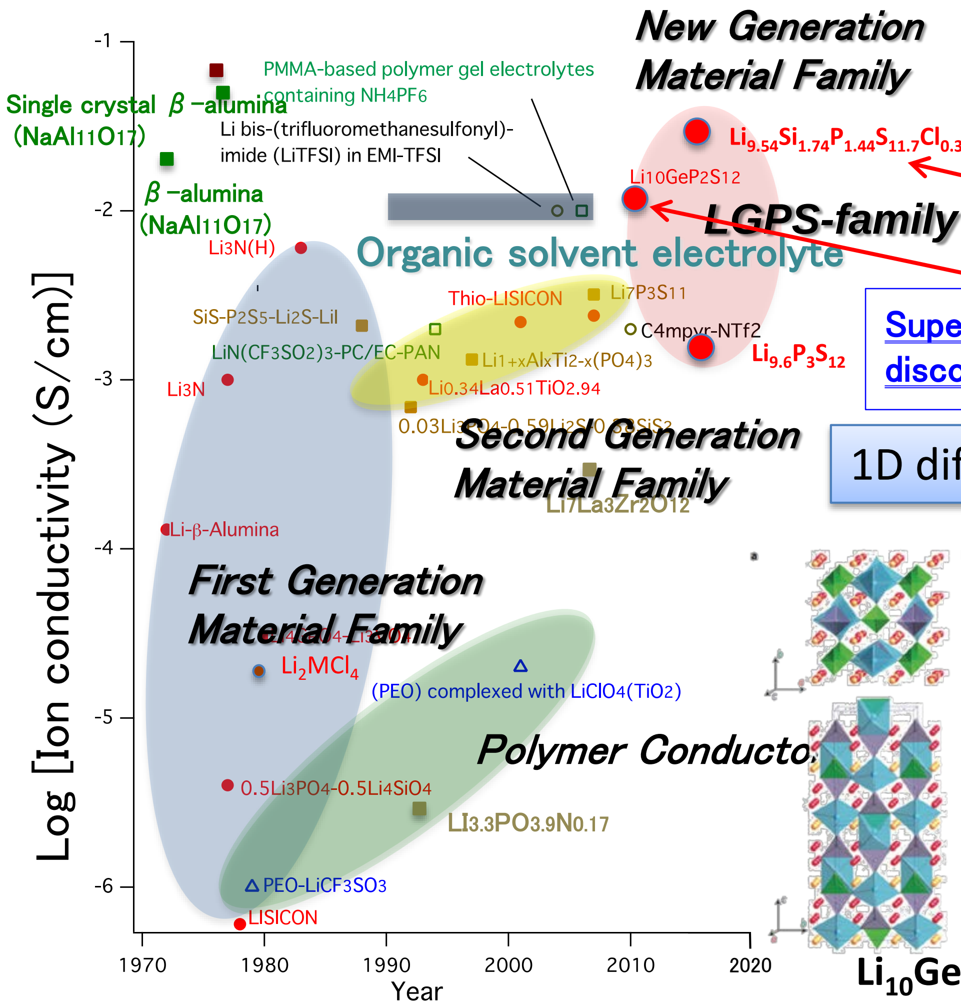
In operando measurement



Energy materials

Development of all-solid ceramic buttery based on new super ionic conductor

Tokyo Inst. Tech, KEK, TOYOTA, Ibaraki Pref.



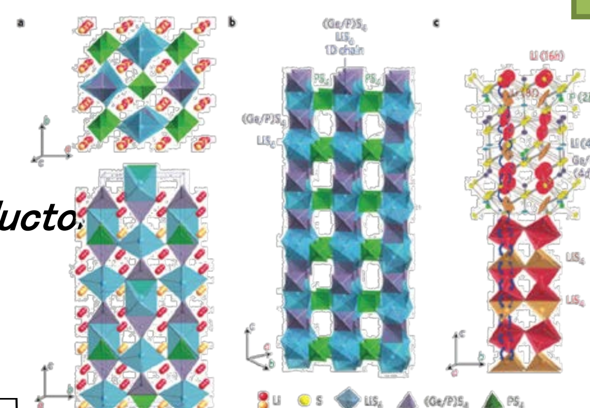
Neutron diffraction have revealed the diffusion path of ions, which is a key for development of new buttery materials.

Super Ionic Conductor discovered in 2011

1D diffusion path

Super Ionic Conductor discovered in 2016

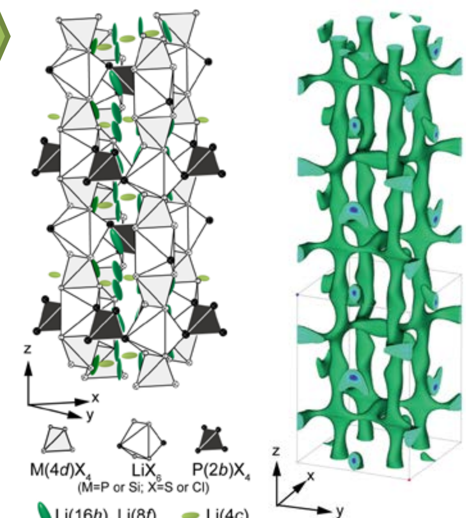
3D diffusion path



$Li_{10}GeP_2S_{12}$

Nature Materials (2011)

450citations for 4 years



$Li_{9.54}Si_{1.74}P_{1.44}S_{11.7}Cl_{0.3}$

Nature Energy (2016)

Newspaper (Tokyo Newspaper (7/25), Chunichi News Paper (7/28))

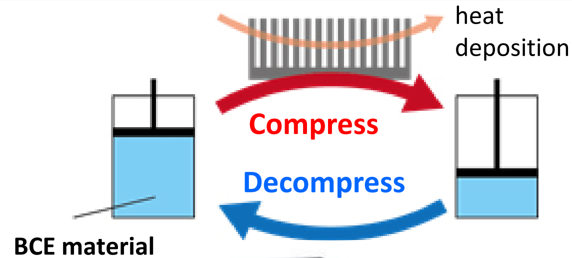
TOYOTA will load all-solid buttery into Electric Vehicle in 2022

Natture **567**, 506 (2019)

Colossal barocaloric effects in plastic crystals

Candidate for new solid-state refrigerant (coolant)

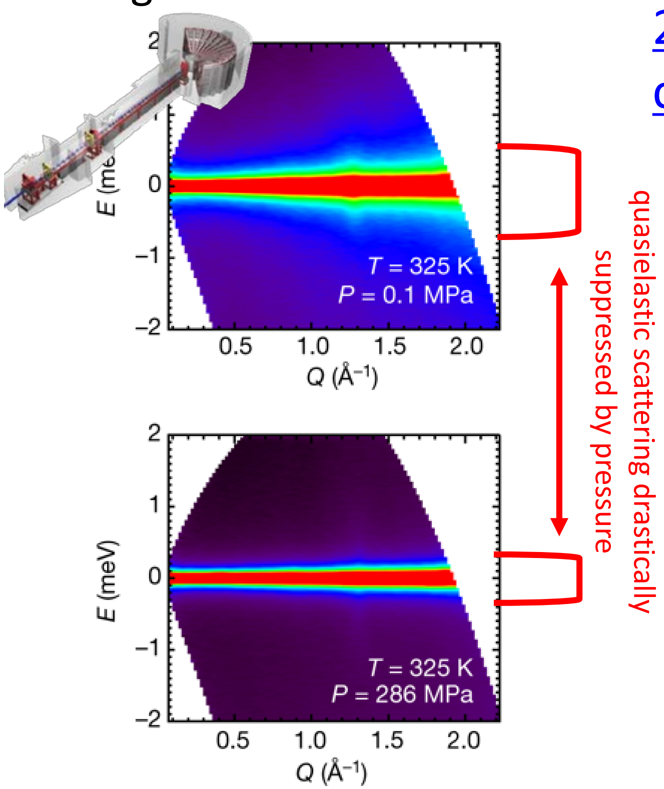
plastic crystal: neopentylglycol (NPG)



- ✓ NPG shows colossal entropy changes by small pressures
- ✓ Colossal barocaloric effect materials can change refrigeration

refrigeration

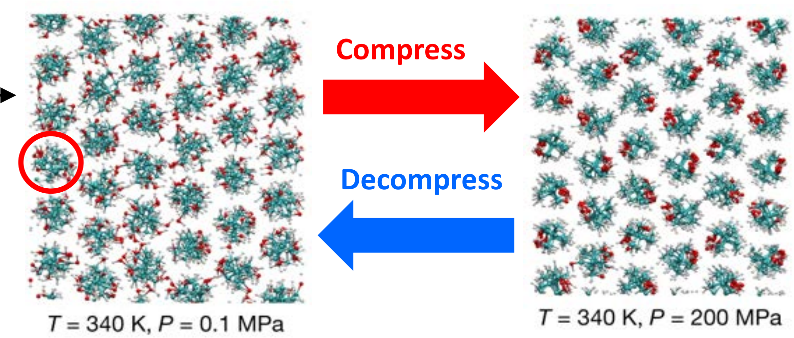
25~30% of electricity consumption is for refrigeration



Microscopic mechanism of colossal entropy changes
Combining MDA calculations, quasielastic neutron scattering experiments under pressures reveled that colossal entropy changes in NPG caused by change of disordering motion in NPG molecules, which is suppressed by even relatively small pressures.

MDA calculations

NPG molecule →



Thank you for your kind attention