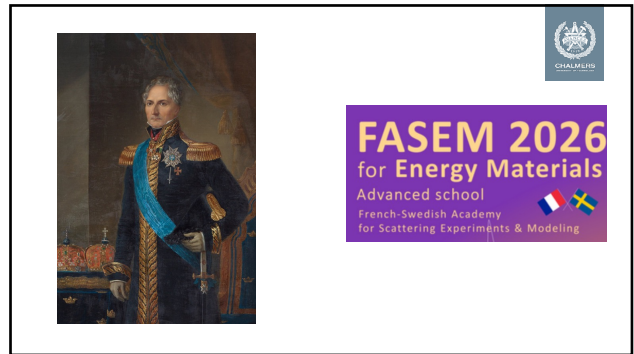
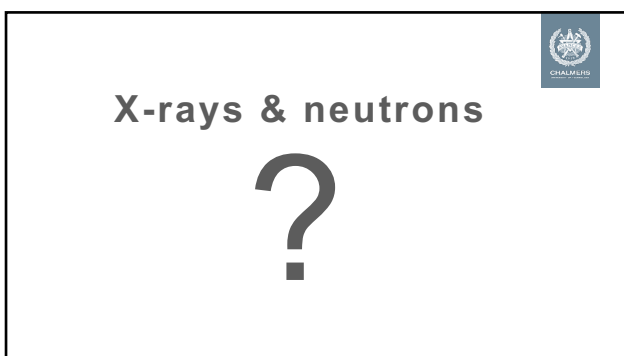


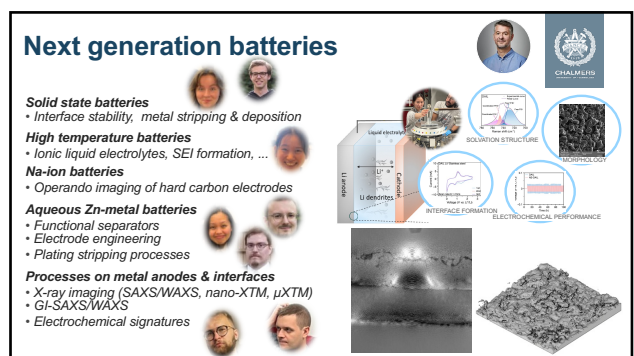
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2



3



4

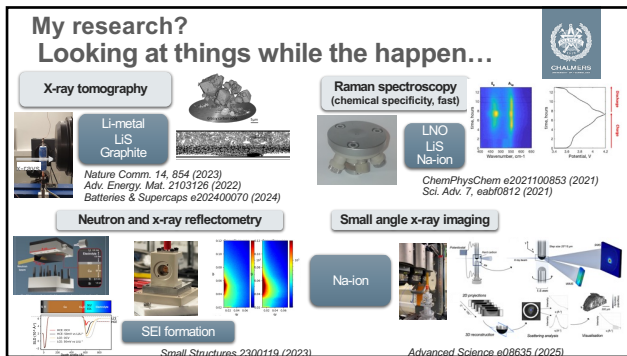
### My research? Looking at things while the happen...

**X-ray tomography**  
Li-metal  
LiS  
Graphite  
*Nature Comm.* 14, 854 (2023)  
*Adv. Energy. Mat.* 2103126 (2022)  
*Batteries & Supercaps* e202400070 (2024)

**Raman spectroscopy  
(chemical specificity, fast)**  
LNO  
LiS  
Na-ion  
*ChemPhysChem* e2021100853 (2021)  
*Sci. Adv.* 7, eabf0812 (2021)

**Neutron and x-ray reflectometry**  
SEI formation  
*Small Structures* 2300119 (2023)

**Small angle x-ray imaging**  
Na-ion  
*Advanced Science* e06835 (2025)



5

to host the  
European  
Spallation Source  
in Scandinavia

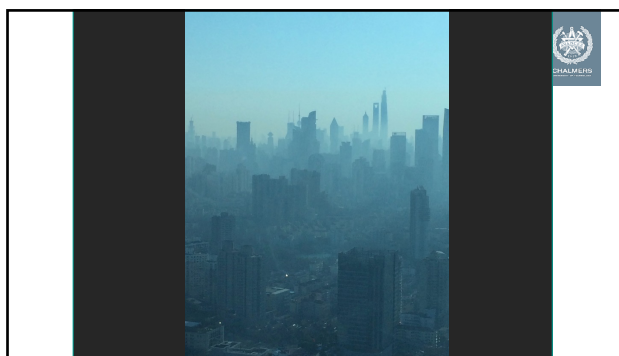
EUROPEAN  
BATTERY  
HUB



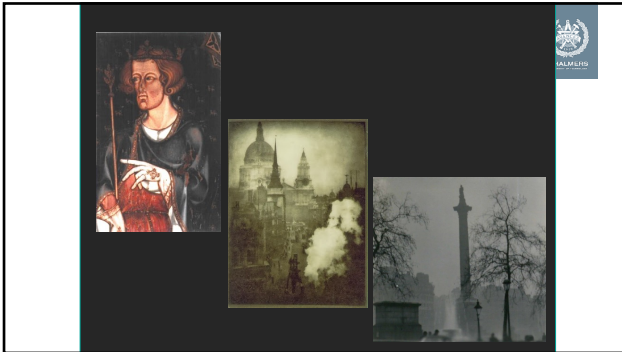
6



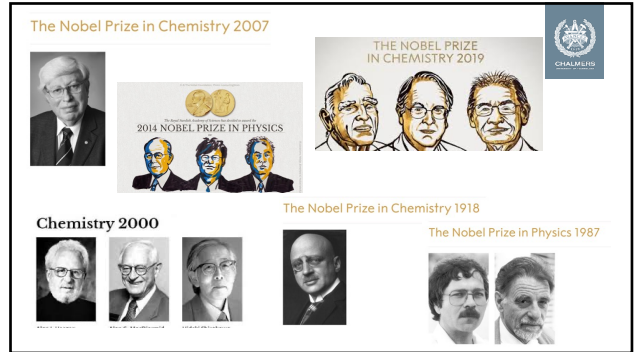
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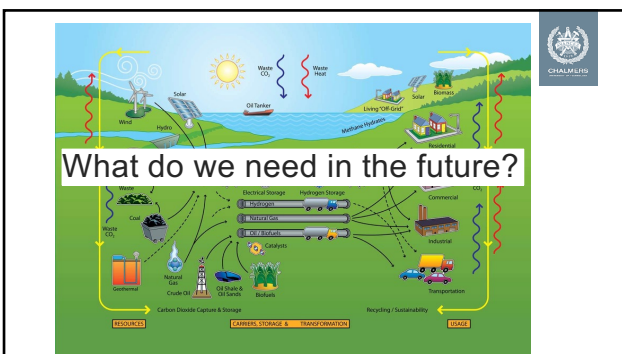
8



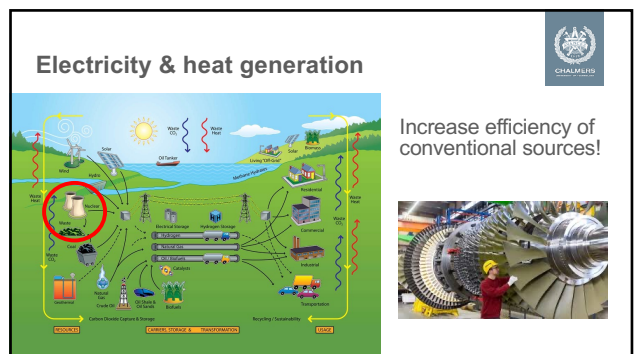
9



10



11



12

### Energy saving...

The Savings...

**11W LED**  
LFE = 25,000 hours per bulb (25 years lifetime)

**60W Incandescent**  
LFE = 1,000 hours per bulb (1 year lifetime)

Thermoelectric generator

TE generator

13

### Electricity & heat generation

Enable future renewable energy systems!

14

### Solar energy harvesting

Best Research-Cell Efficiencies

Efficiency (%)

1950 1960 1970 1980 1990 2000 2010 2015

Legend:

- Single-junction Silicon
- Thin-film (CdTe, Si, a-Si)
- Multi-junction (GaAs, InGaP, InGaAs, Ge)
- Organic
- Perovskite
- Quantum dot
- Hybrid
- Other

15

### Electricity transfer

Can we reach 1 MV?

16

### Fuel cells – catalysis, ion transport, storage

Hydrogen storage gets real  
CHEMISTRYWORLD Aug 2019

17

### Energy storage & conversion

18

### Energy storage & conversion 100 years of development....

19

### Energy storage & conversion

OCTOBER 27, 1934 NATURE 657

"I feel that if it were possible for those far-seeing men who founded this Institution to come amongst us to-day, they would consider that the great heritage which they left us has been fully preserved."

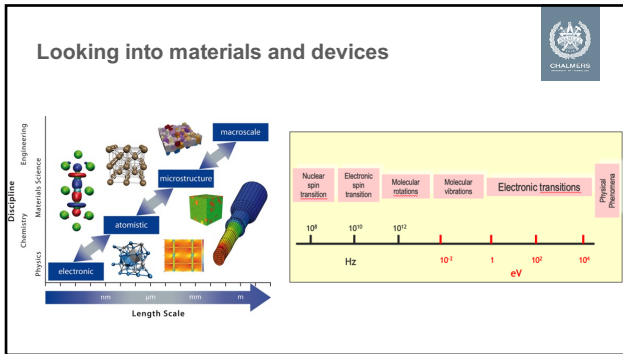
**Training of Mercantile Marine Officers**

Some important recommendations for the better training of apprentices for sea service are contained in a report just issued by an Advisory Committee to the Maritime Committee of the Shipping Federation. To qualify for the position of a junior officer in the British Mercantile Marine, it is necessary to serve an apprenticeship of four years, or three years if a boy has passed through the *Commerce*, or *Mariner*, or *Peabody* College, and to pass the Board of Trade examination for second mate. At present, there is no recognized course of instruction or any uniformity in training for apprentices or mates, and very often it is only with the greatest difficulty that apprentices prepare themselves for examination. Some shipping companies have special schemes of training; but such is not the general case. It is now proposed that a Central Board of Control should be set up with the power to draw up a standard syllabus of instruction, to set annual examination papers, to give practical advice to captains of ships in matters of education, to appoint local boards of examiners and to publish periodical statistics relating to the

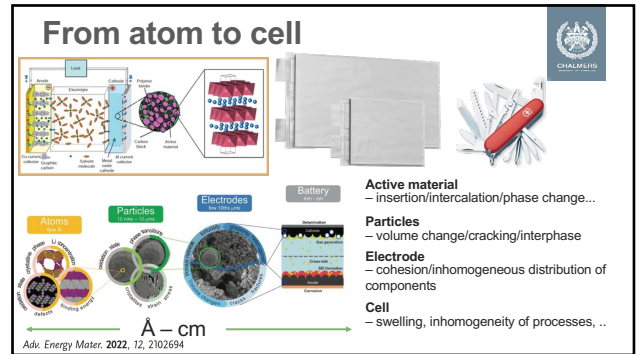
**Battery-Electric Cars**

After many years of almost suspended animation, the battery-electric vehicle industry is showing signs of life. At the Exide motor show, Mr. D. P. Burns stated that the monthly output of these vehicles in Great Britain is larger than it has ever been before. Compared with petrol vehicles, they make less noise and produce less atmospheric pollution. Statistics prove that their life is much longer and their maintenance is much less than that of any other form of mechanically propelled road vehicle. Several corporations are using electric vans in connection with their electrical apparatus hiring schemes. The West Ham undertaking has vans with a speed of 20 miles per hour and a range of 60 miles per charge. They use an electric motor coupled to the back-axle through differential gearing. The charging arrangements are quite simple: a "jack" is provided on the dashboard for connecting with the mains and there is an automatic control to limit the rate of charging. This undertaking has introduced a night tariff of 6d. per unit for vehicle charging. In certain cases, such vehicles will prove more economical than petrol vans,

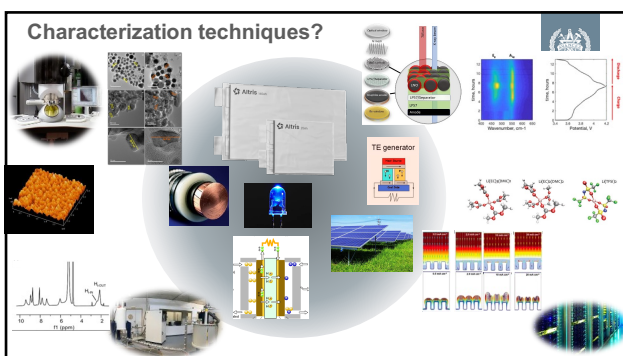
20



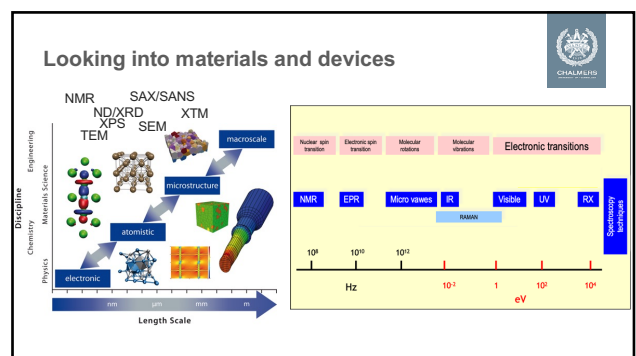
21




22



23




24



# X-RAYS & NEUTRONS?

25

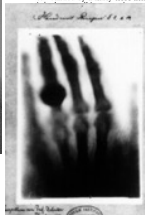
## X-rays?



**ON A NEW KIND OF RAYS!**

**A** DISCHARGE from a large induction coil is passed through a Hittorff's vacuum tube, or through a well-evacuated connect of Lemblin's tube. The tube is surrounded by a fairly close-fitting shield of black paper, which is entirely disconnected from the tube. When brought near, whether the painted surface be of barium platinocyanide, or of any other substance, a fluorescence is observed, which is quite opaque to light. It is therefore, transparent, but in its paper is very translucent, printer's ink, or a single card does not prevent the fluorescence from appearing. So, again, a shadow on the paper is produced, and a sheet of aluminium, 15 centimetres thick, is still called the rays.



- From the *Stratford*, 1895.



*NATURE* [January 23, 1896]


26

## Neutrons?

692

*The Existence of a Neutron.*




§ 1. It is found that the rays from a source of radioactivity bombard the material.

Proceeding


27

## X-rays & neutrons




### X-rays

- Electromagnetic waves
- $\lambda = 0.1-100 \text{ \AA}$  ( $E = 120 \text{ eV} - 12 \text{ keV}$ )
- Interact with the electrons in the material



### Neutrons

- Subatomic particles
- Interact with atomic nucleus
- No "free" neutrons



$$E = \frac{1}{2}mv^2 = \frac{h^2}{\lambda^2 m} = \frac{81.81}{\lambda^2}$$

- By changing their velocity we can get  $\lambda \approx 1-30 \text{ \AA}$  (80-0.1 meV)

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### X-rays & neutrons

**Neutrons:**

- Scatter – elastically
- inelastically
- Absorbed

**X-rays:**

- Scatter – elastically
- inelastically
- Absorbed
- Excite core electrons – photoelectrons

Roger Pynn: Neutron scattering – a primer Los Alamos 1990

29

### Scattering experiment

In the experiment we measure the double differential scattering cross section

$$\frac{d^2\sigma}{d\Omega d\omega}$$

total scattering cross section  $\sigma_{tot} = \sigma_e + \sigma_a + \sigma_T$

**Dynamic structure factor**

$$\frac{d^2\sigma}{d\Omega d\omega} \propto \int dt \int d\mathbf{r} e^{-i(\omega t - Q \cdot \mathbf{r})} (\rho(\mathbf{r}, 0) \rho(\mathbf{r}' + \mathbf{r}, t)) = S(Q, \omega)$$

$$g(\mathbf{r}, t) = \frac{1}{N} \int d\mathbf{r}' (\rho(\mathbf{r}, 0) \rho(\mathbf{r}' + \mathbf{r}, t))$$

$g(\mathbf{r}, t) \Leftrightarrow S(Q, \omega)$  (Fourier transforms)

30

### Characterization techniques

EPI Web of Conferences 188, 05001 (2018)

31

### X-RAYS FOR MATERIALS SCIENCE

32

### Neutrons for materials science

- Fission in a nuclear reactor
- Spallation process – bombardment with protons

The slide illustrates the production of neutrons for materials science. On the left, 'Spaltung' (fission) is shown with a diagram of a nuclear reactor core and a photograph of a reactor building. On the right, 'Spallation' is shown with a diagram of a proton beam hitting a target to produce neutrons, and a photograph of a spallation neutron source facility. A central map shows the locations of various neutron facilities across Europe and North America.

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### X-ray and neutron facilities for materials science

This slide highlights the interdisciplinary nature of materials science research. A central diagram shows a 'Length Scale' axis from atomic to macroscopic, with corresponding disciplines: Physics (electronic), Chemistry (atomic), Engineering (microstructure), and Materials Science (macroscale). Surrounding this are images of X-ray diffraction patterns, molecular models, and material microstructures. Citations include 'Int. J. Mat. Sci. 2020, 11, 7275 5 of 15' and 'Nature (2015), 527, 349'.

34

### X-rays

A map of Europe shows the locations of major X-ray synchrotron facilities: MAXIV (Sweden), PETRA III (Germany), SLS/PSI (Switzerland), and ESRF (France). A central diagram shows a network of user facilities. The text 'User facilities – best science' is at the bottom.

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### Neutrons

A world map shows the locations of major neutron facilities: ILL (France), ISIS (UK), ESS (Sweden), SINQ (Switzerland), and J-PARC (Japan). A central diagram shows a network of user facilities. The text 'User facilities – best science' is at the bottom.

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Contributing to the development of society!

*sustainability*  
*health*  
*energy*

— tackling global challenges with research infrastructures!

37

Contributing to the development of society!

From virtual screens to promising inhibitors of coronaviruses:  
An effort to develop an antiviral drug to treat COVID-19

**JACS**  
Journal of the American Chemical Society

**Ultralarge Virtual Screening Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses**  
Andreas Lattner, Hektor Gullberg, Eldar Abubakirov, Chey Chee Yee, Daria Akhmetova, Vladimir O. Sokolov, Yashika Madhavan, Lucas Vargas, Sumit Dha Jung, Dik Jochmans, Janina Krennrich, Ali Tay, Do Luong, Yixi Guo, Alexander J. Cook, Yousuf Akbar, Olga Ivanenko, Ludovic W. E. Monier, Mir-Landjung Martin, J. van Veen, John Korte, Johan Lennestrand, Jan Kårlberg, Kristian Svanberg, U. Hakan Dursun, and Jens Carlsson\*

*Chem. Sci., An Open Access Article. Published on 2022. Downloaded on 2/22/2023 11:02:02 AM.*

38

Using neutrons to look into materials

**Resonant Scattering in Samarium and Gadolinium**  
B. W. ROBERTSON and D. G. HIND  
Atomic Energy Project, National Research Council of Canada,  
Chalk River, Ontario, Canada  
(Received June 21, 1951)

**SAMARIUM**—Scattering of low energy neutrons by samarium has been investigated by the method outlined in the preceding paper.

Physical Review 83, 841 (1951)

PHYSICAL REVIEW VOLUME 83, NUMBER 2 JULY 14, 1951

**Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances**  
C. G. SHULL, W. A. STANTON, and E. O. WINEAR  
National Bureau of Standards, Washington, D. C.  
(Received March 16, 1951)

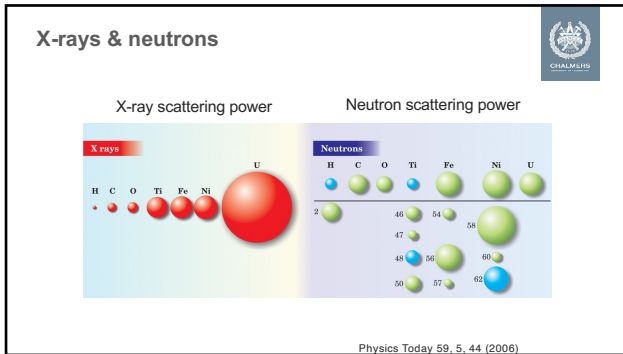
Neutron scattering and diffraction studies on a wide variety of paramagnetic and antiferromagnetic substances are reported in the present paper. The paramagnetic diffuse scattering method of Shull and Stinson has been applied, together with the determination of the magnetic form factor for  $\text{Ni}^{2+}$  ions. From the form factor

Physical Review 83, 334 (1951)

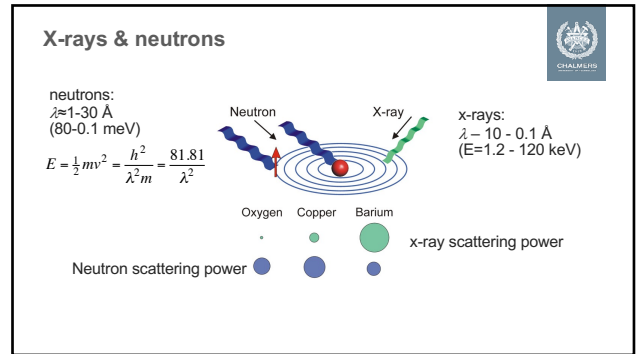
39

X-RAYS OR NEUTRONS?

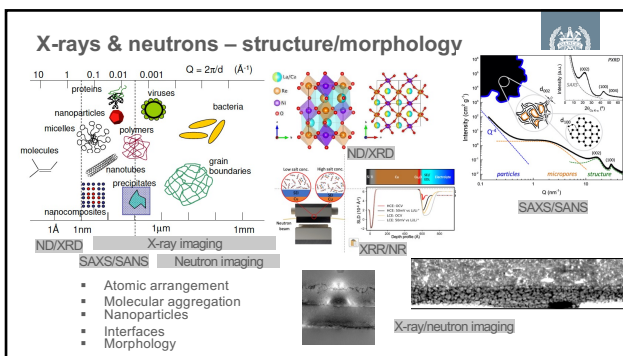
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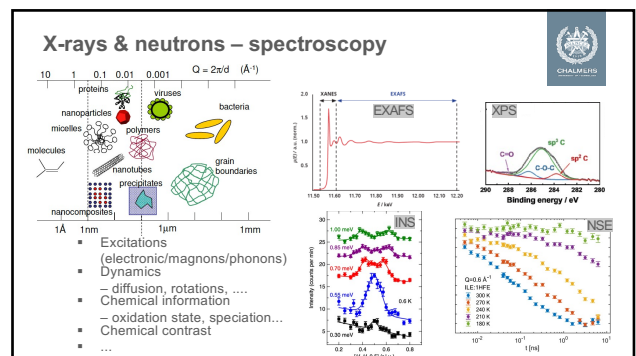
41



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## X-RAYS AND/OR NEUTRONS! (or not at all...)

- Contrast?
- Time- & length scale of the process?
- Spatial & temporal resolution required?
- Size of the beam?
- Possibility for a relevant environment?
- .....





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## Case study – batteries!


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CELL                  MODULE (x4)                  PACK (x48)

MODULARITY — FLEXIBILITY — OPTIMISATION

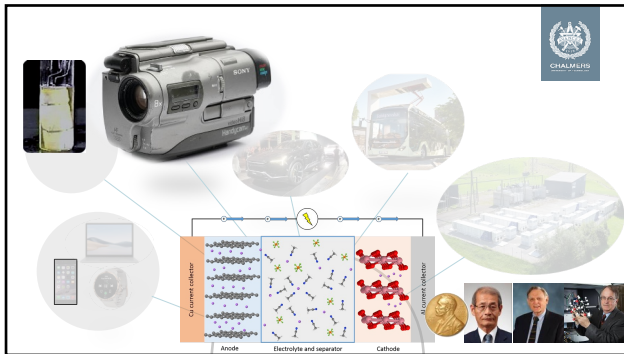
47



CELL                  MODULE (x4)                  PACK (x48)

MODULARITY — FLEXIBILITY — OPTIMISATION

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### X-rays and neutrons for batteries

#### LOOKING INTO MATERIALS

structure/morphology/dynamics/functionality

#### LOOKING INTO DEVICES

processing/products/operation

50

### Material – component – cell

Adv. Energy Mater. 2022, 12, 2102694

51

### “Atomic level” – structure of material

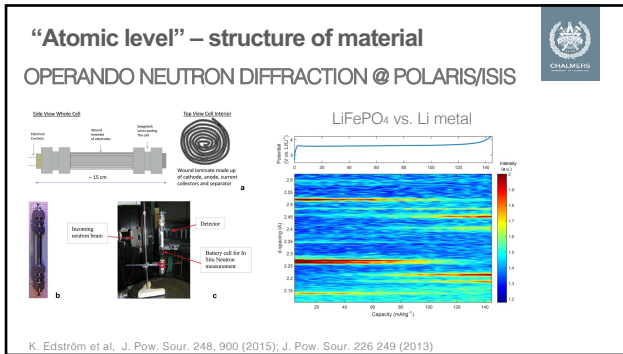
A NEUTRON DIFFRACTION STUDY OF THE FERRIMAGNETIC SPINEL  $\text{NiCo}_2\text{O}_4$

F. D. Battle and A. K. Cheetham  
Chemical Crystallography Laboratory, 9 Parks Road, Oxford OX1 3PD

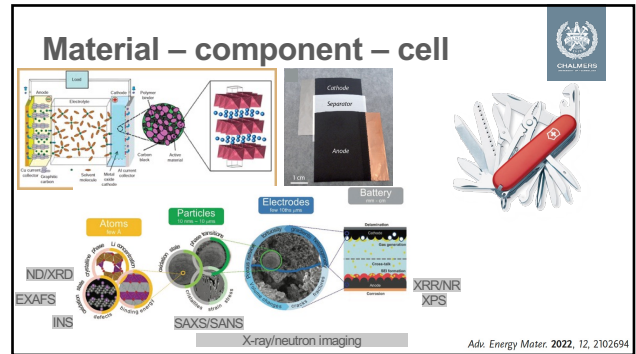
J. B. Goodenough  
Inorganic Chemistry Laboratory, South Parks Road, Oxford, OX1 3QR

Mat. Res. Bull. Vol. 14, pp. 1013–1024, 1979. Printed in the USA.  
0025-5408/79/081013-12\$02.00/0 Copyright (c) 1979 Pergamon Press Ltd.

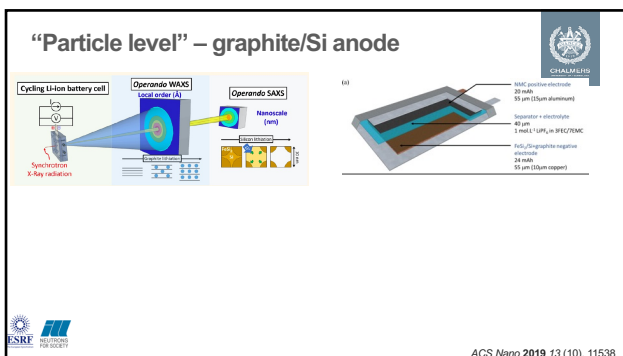
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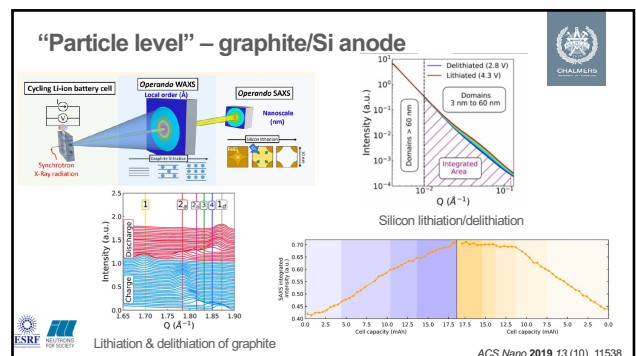
53



54



55



56

### "Particle level" – inhomogeneous lithiation

- Fluorescence X-ray microscopy following lithiation of LFP particles

57

### "Particle level" – inhomogeneous lithiation

Lithiation of LFP cathode – all particles are not lithiated at the same time

58

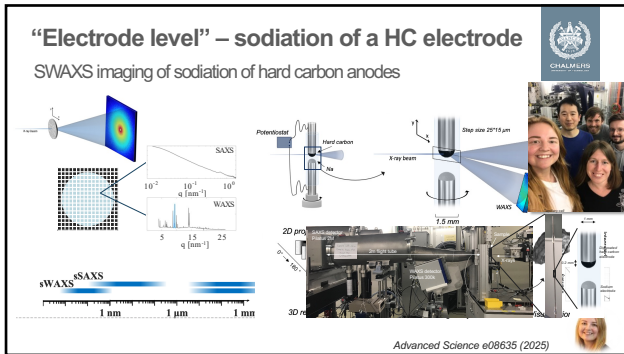
### Material – component – cell

59

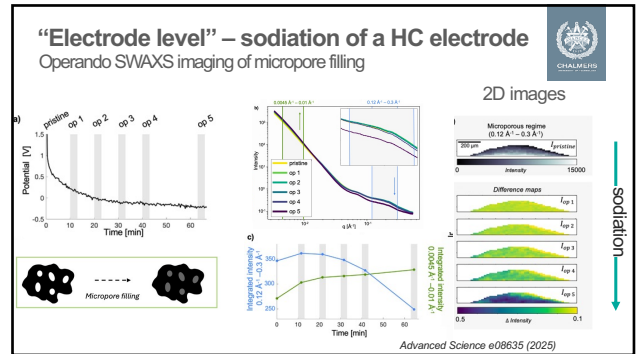
### "Electrode level" – sodiation of a HC electrode

SWAXS imaging of sodiation of hard carbon anodes

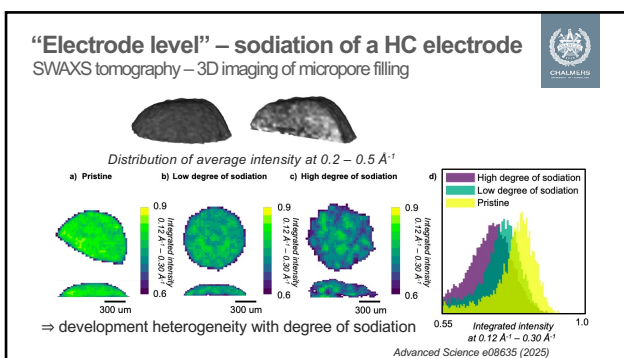
60



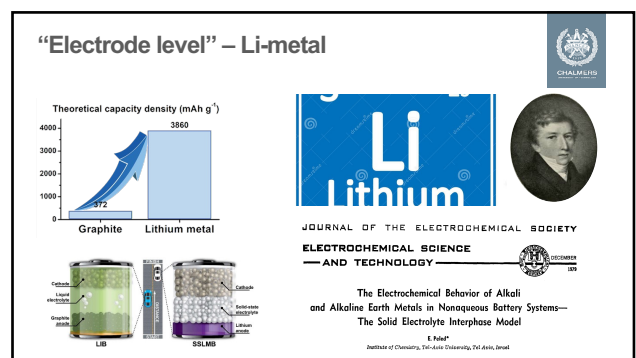
61



62



63



64

### “Electrode level” – Li-metal

- Operando XTM @ TOMCAT SLS/PSI (CH)
  - 50 s / tomogram
  - 0.325  $\mu\text{m}$  voxel size,  $\sim 1.0 \mu\text{m}$  resolution

832  $\mu\text{m}$

- Counter electrode (Li-metal)
- Electrolyte (liquid)
- Working electrode (Cu-pin)
- Plated Li (black)
- Electrolyte (grey)
- Cu pin (light grey)

TOMCAT X02DA  
PSI  
Nature Comm. 14, 854 (2023)

65

### “Electrode level” – Li-metal

#### Nano-tomography

- $\approx 1 \text{ min/tomo}$  (3D) single distance
  - *operando experiments*
- phase contrast imaging  $\approx 8 \text{ min/tomo}$ 
  - *in situ/ex situ experiments*

ID16B ESRF  
Voxel size 50 nm/resolution  $\approx 150 \text{ nm}$

chemrxiv-2025-wf4wx-v2  
EUROPEAN BATTERY HUB, ESRF, c2a, litem, c2a, irig

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### “Electrode level” – Li-metal

#### Growth of Li structures

6 min    12 min    24 min    60 min

20  $\mu\text{m}$

EUROPEAN BATTERY HUB  
chemrxiv-2025-wf4wx-v2

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### “Electrode level” – Li-metal

200 kPa – 6 MPa

38.5 mm

4 mm

Bulk Li  
Calgard separator  
Deposited Li  
Bulk Li

760 kPa  
180 kPa

Porosity 1<sup>st</sup> cycle:  
760 kPa – 3.2%  
180 kPa – 18 %

EUROPEAN BATTERY HUB

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### What to do with more neutrons/photons?

Bright sources & small beams:

- Precise data
- Nanocrystals
- Fast experiment
  - screening
  - kinetics, reactions
  - spatial scanning
- Complex samples/environment
  - operando
  - processing

Acc. Chem. Res. 51, 290 (2018)  
ACS Energy Lett. 3, 356 (2018)  
Chem. Rev. 117, 13123 (2017)

74

### What to do with more neutrons/photons?

Bright sources & small beams  
X-ray Imaging

- Image extended sample volume with high resolution
- Flexibility on sample environment
- Combined modalities

Acc. Chem. Res. 51, 290 (2018); ACS Energy Lett. 3, 356 (2018); Chem. Rev. 117, 13123 (2017)

75

### What do we need for 2030+?

Fundamental discoveries

Materials & devices in action

- Instrument development
- Dedicated sample environments
- Workflows & data infrastructure
- Complementary infrastructure
- Linking academy, industry & facilities
- User support & training
- Access

Education

Innovation

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**PERSPECTIVE**

ACCELERATING BATTERY CHARACTERIZATION USING NEUTRON AND SYNCHROTRON TECHNIQUES: TOWARD A MULTI-MODAL AND MULTI-SCALE STANDARDIZED EXPERIMENTAL WORKFLOW

Duncan Atkins, Ennio Capria, Kristina Edström, Theodosios Famprikis, Alexis Grimaud, Quentin Jaquet, Mark Johnson, Aleksandar Matic, Paul Norby, Harald Reichert, Jean-Pascal Rueff, Claire Villeveuille, Marnix Wagemaker,\* and Sandrine Lyonnard\*

Battery Interface Genome - Materials Acceleration Platform

BATTERY 2030

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**EUROPEAN BATTERY HUB**

The battery hub at ESRF: accelerating and standardizing battery characterization workflows

Coordinator : S. Lyonnard

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The battery hub at ESRF: accelerating and standardizing battery characterization workflows

**The batteryhub project**  
 WPO - Coordination IRIG  
 Multiparameter Correlative characterization

**WP1. Na-ion**  
 1.1 Reaction and degradation mechanisms in liquid-based Na-ion cathodes and anodes  
 1.2 Towards stable high energy cathodes and enhanced composite anodes

**WP2. ASSB**  
 2.1 Control of new organic/inorganic electrolytes & catholytes  
 2.2 Towards a stable anode-free battery

**WP3. Synchrotron-based workflows & methods**  
 3.1 New techniques, methods & tools  
 3.2 Transferability to new topics and communities

**WP4. Towards an all-solid state Na battery**

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The battery hub at ESRF: accelerating and standardizing battery characterization workflows

**The batteryhub project**  
 WPO - Coordination IRIG  
 Multiparameter Correlative characterization

**WP1. Na-ion**  
 1.1 Reaction and degradation mechanisms in liquid-based Na-ion cathodes and anodes  
 1.2 Towards stable high energy cathodes and enhanced composite anodes

**WP2. ASSB**  
 2.1 Control of new organic/inorganic electrolytes & catholytes  
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**WP3. Synchrotron-based workflows & methods**  
 3.1 New techniques, methods & tools  
 3.2 Transferability to new topics and communities

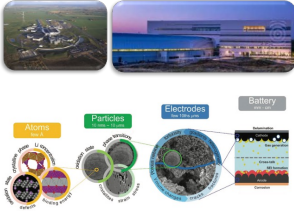
**WP4. Towards an all-solid state Na battery**

**New way of working!**


- Community driven approach
- sharing of ideas, beam time & data
- develop and share methodology, sample environment & analysis tools
- bring new capabilities to the facility

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### Neutrons & X-rays for energy materials research – role of large-scale facilities



- From atom to device
  - length scales
  - time scales
  - chemical sensitivity
  - operando
- Critical mass for method development
- Cost effective user support & training
- Resources for handling big data, data sharing & AI/ML
- Focal point for the community



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### In 2040....



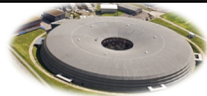
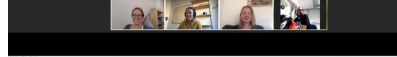
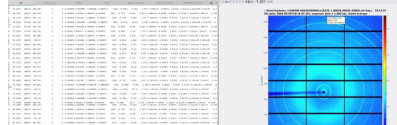

- How do we access facilities?
- How are we doing experiments?
- What do we need in terms of support?
- How do we work with data?

this ... and not this ...






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**IS THIS THE NEW BLACK?**



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**Chalmers:**

- Martina Olsson
- Josef Rizell
- Marita Afandika
- Quan Wu
- Andreas Erlandsson
- Elin Dufvenius

**SLS/PSI:**

- Federica Marone
- Manuel Guizar Sicaïros

**CEA/Grenoble:**

- Victor Vanpeene
- Sandrine Lyonnard

**ESRF:**

- Jakub Drnec
- Valentin Vinci
- Olga Stamatî
- Gustavo Pinzon Forero

**MAXIV:**

- Thorbjørn Erik Køppen Christensen
- Innokenty Kantor












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