Neutrons & Muons for Sustainability [Energy]

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KTH Royal Institute of Technology
Stockholm, Sweden

Sustainability - General View

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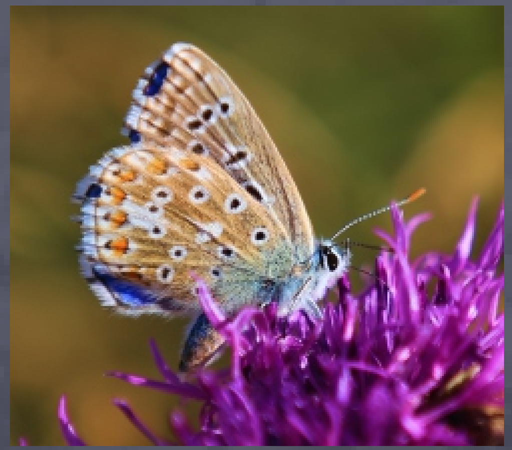

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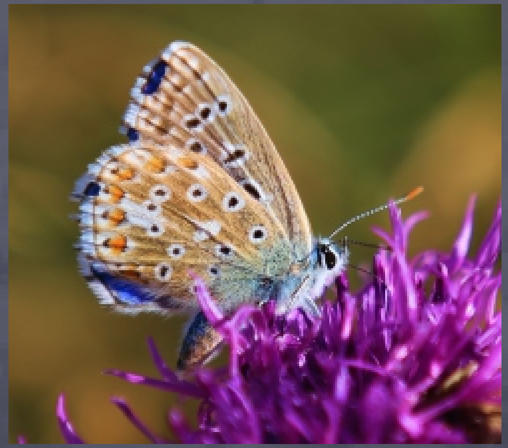

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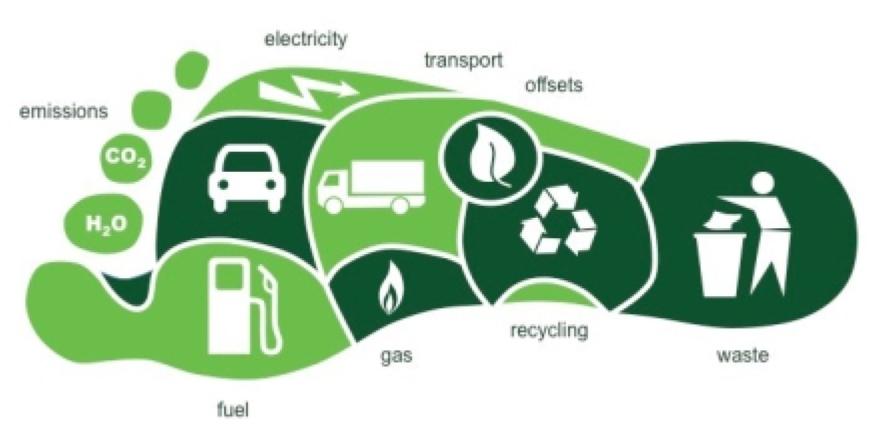

Sustainability - General View

PARIS2015
UN CLIMATE CHANGE CONFERENCE
COP21·CMP11

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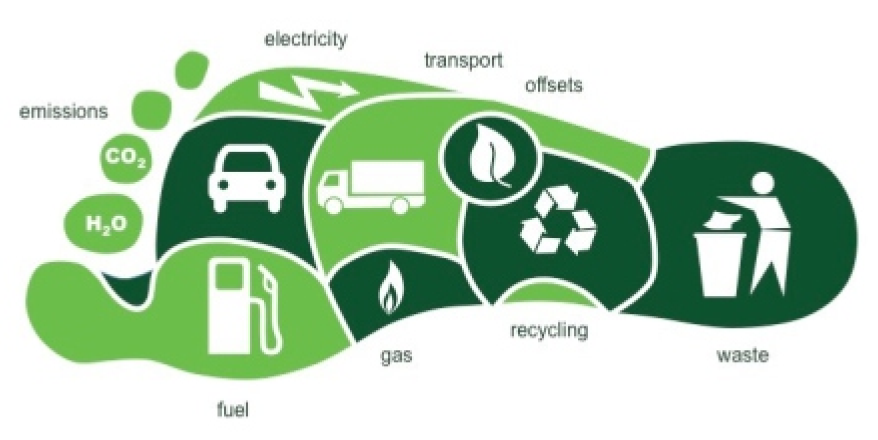


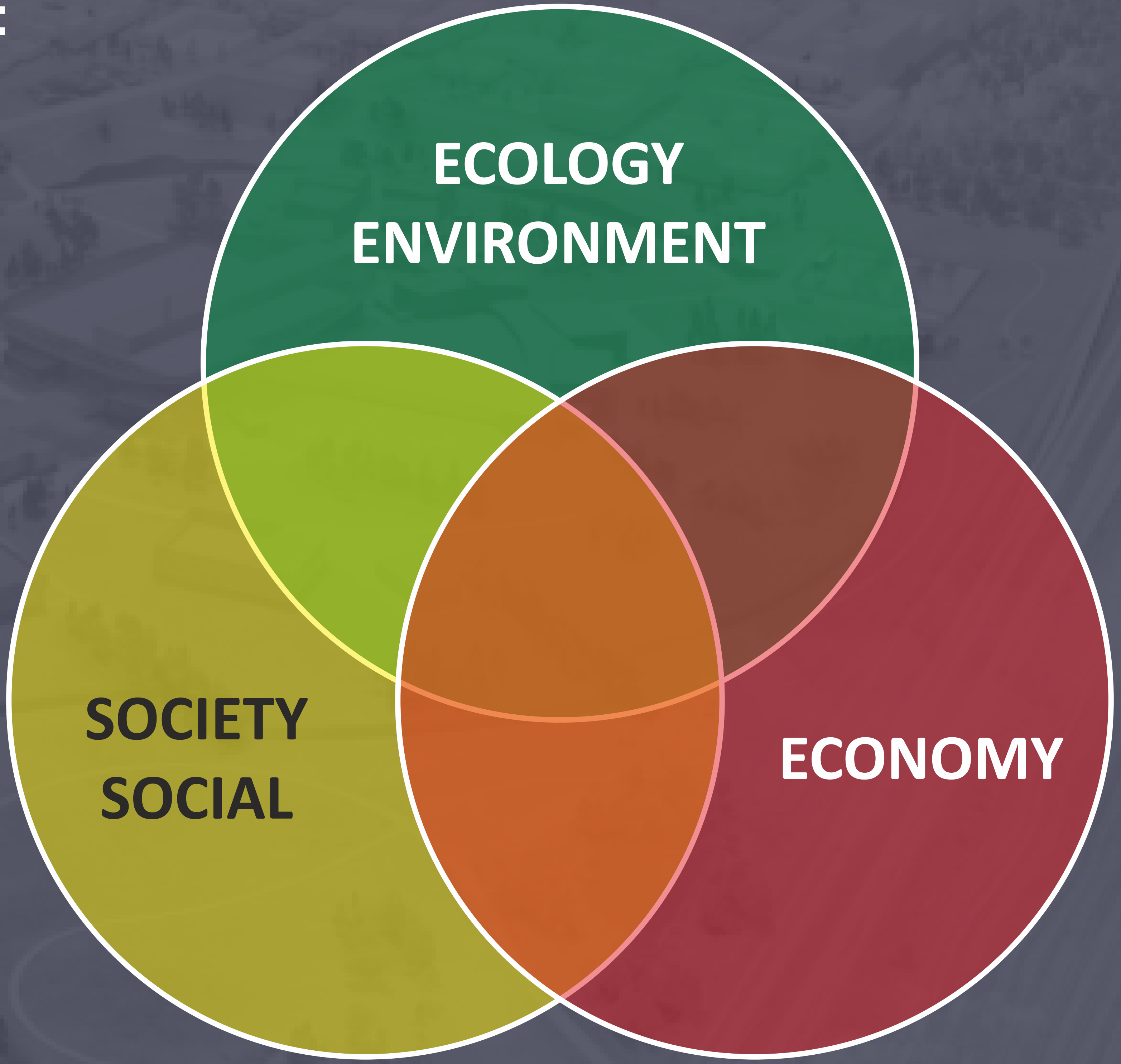
Sustainability - GREEN View

Generally people think about ecology and the environment.

__But this is not the full story__...

Sustainability - Current Definition

- Three pillars/spheres (circles?) of sustainability are:
  - **Ecology/Environment:** Careful use of natural resources, protecting bio diversity, green energy + efficiency, waste management etc.
  - **Society/Social:** Respecting human rights, standard of living, respecting the laws, job security, equal rights/opprotunities, health & health care...
  - **Economy:** Promoting innovation, capital efficiency, local economies, growth enhancement, creating jobs, work against bribery and cartels...

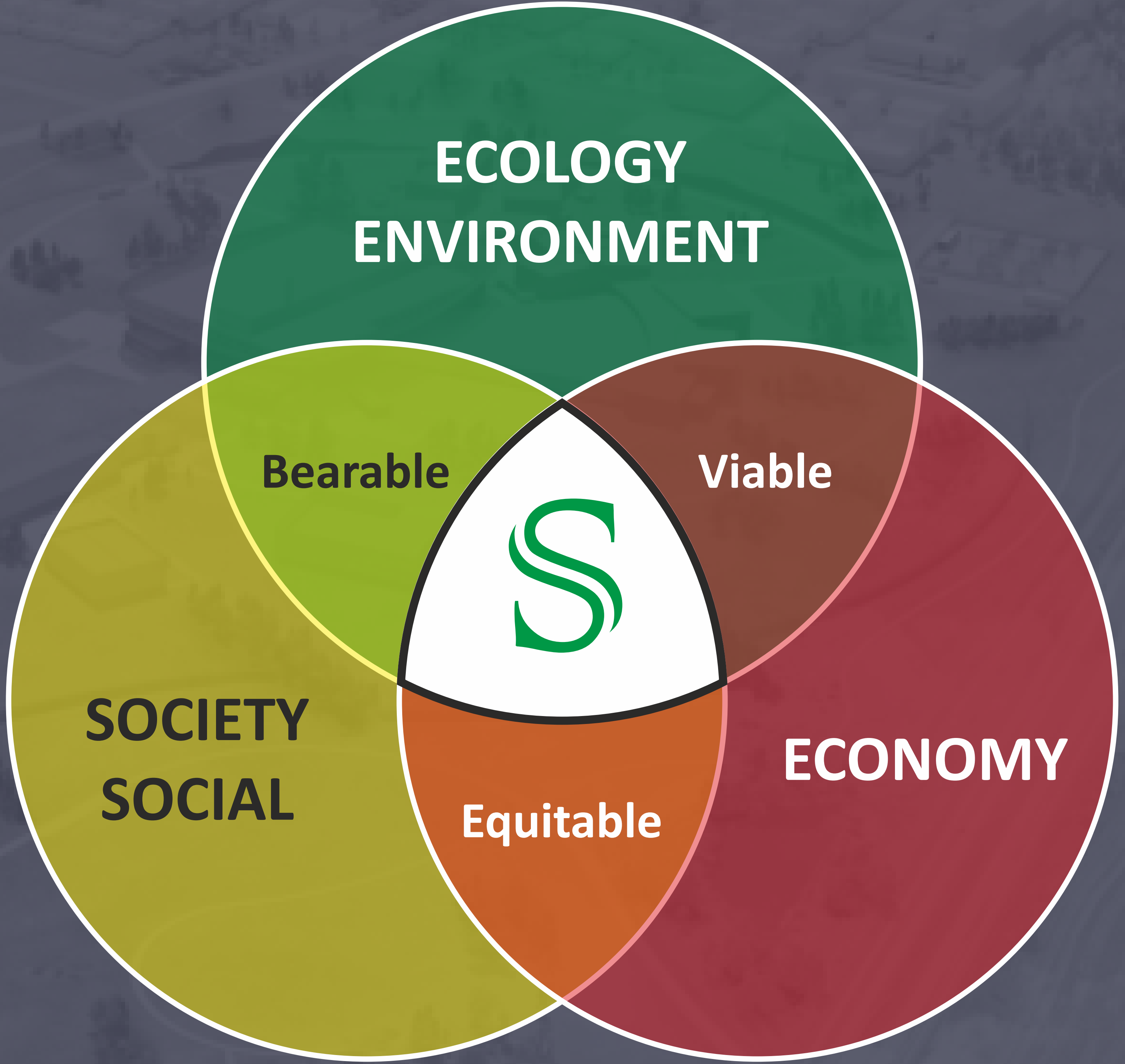


Sustainability - Current Definition

- Only at the intersection of the three you can reach "true" sustainability.

- Further 3 different sub-areas are usually identified fulfilling "2-out-of-3"

- Here one should notice that what previously was "Sustainability" has at some point been transformed into "Sustainable Development"



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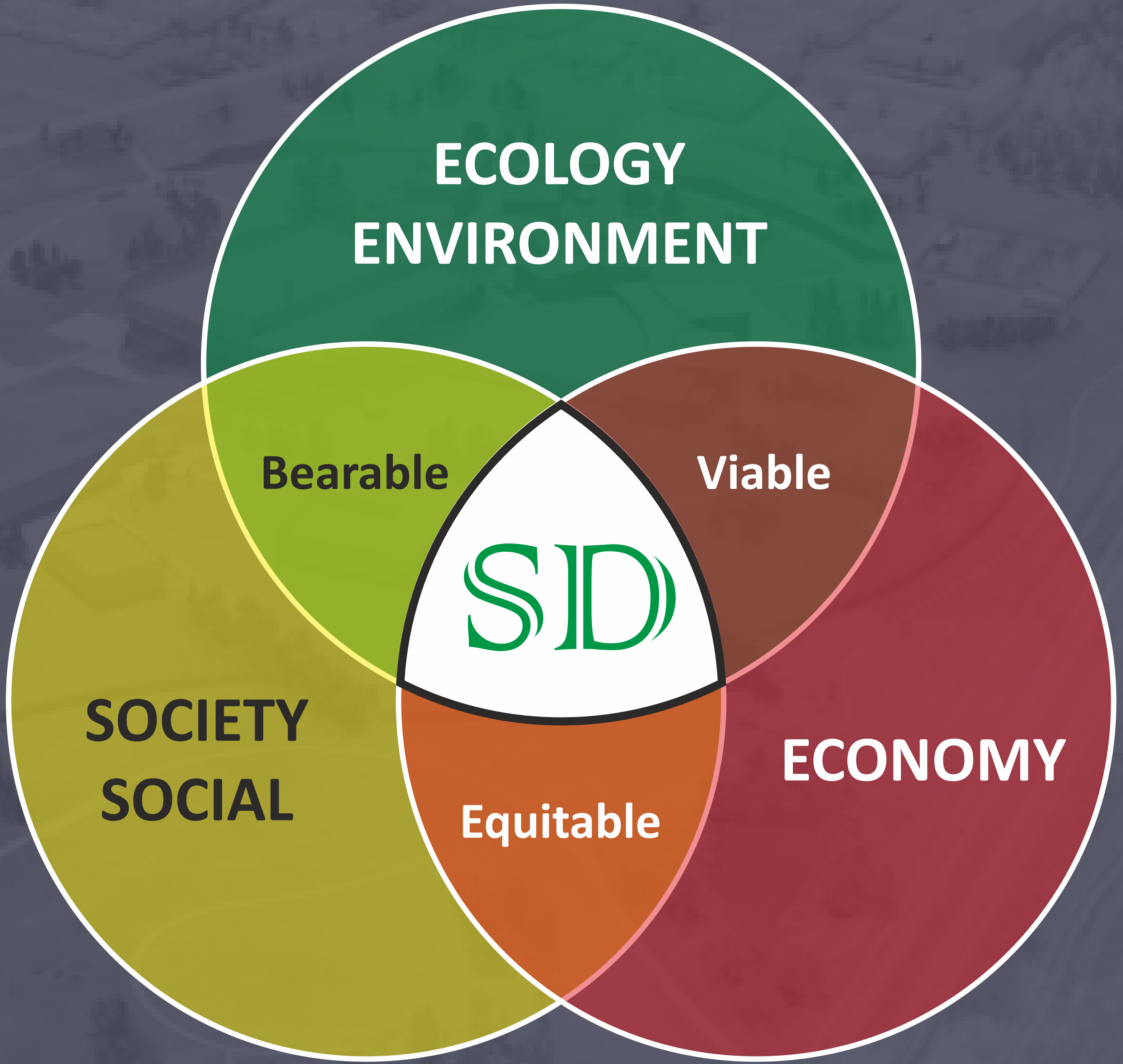
Sustainable Development

- Only at the intersection of the three you can reach “true” sustainability.
- Further 3 different sub-areas are usually identified fulfilling “2-out-of-3"
- Here one should notice that what previously was “Sustainability” has at some point been transformed into “Sustainable Development”
- This is now not anymore a definition for the “best of the planet” but a way to “justify” the presence of our current society (i.e. “ourselves”).



ECOLOGY
ENVIRONMENT

Bearable

Viable

SD

SOCIETY
SOCIAL

ECONOMY

Equitable

Sustainability of the Earth

- Age of the earth: 4.54 ± 0.05 billion years
- Humans have been around for 200 000 years
- That is about 0.004% of the earth's life-time

Worst Case Scenario

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Worst Case Scenario

- Human population is eradicated and then what?
- How is the situation in another 4.5 billion years?

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Worst Case Scenario

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Voluntary Human Extinction Movement

http://www.vhemt.org/

“May we live long and die out”

P.S
I am not supporting this !!! :-D

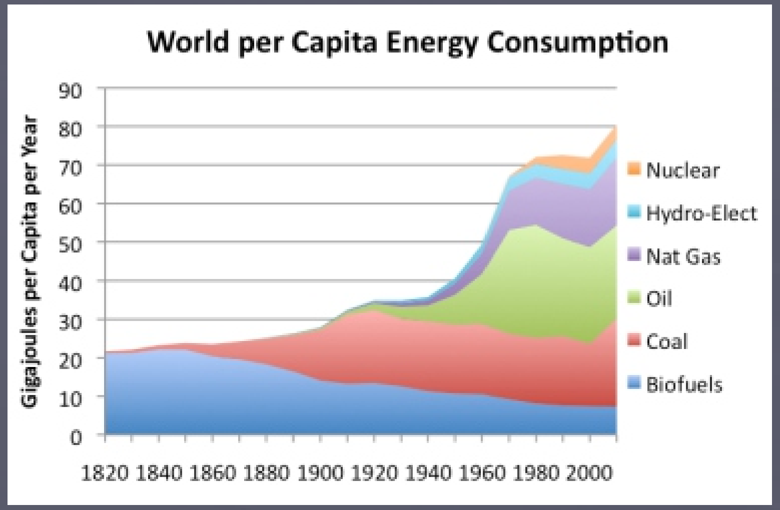
Sustainability of Human Life

- Age of the earth: 4.54 ± 0.05 billion years
- Humans have been around for 200 000 years
- That is about 0.004% of the earth’s life-time

Worst Case Scenario is of course unacceptable !!!

- We really need to start thinking and acting in order to create a sustainable society...
- **How can neutron scattering help ???**

The Energy Problem



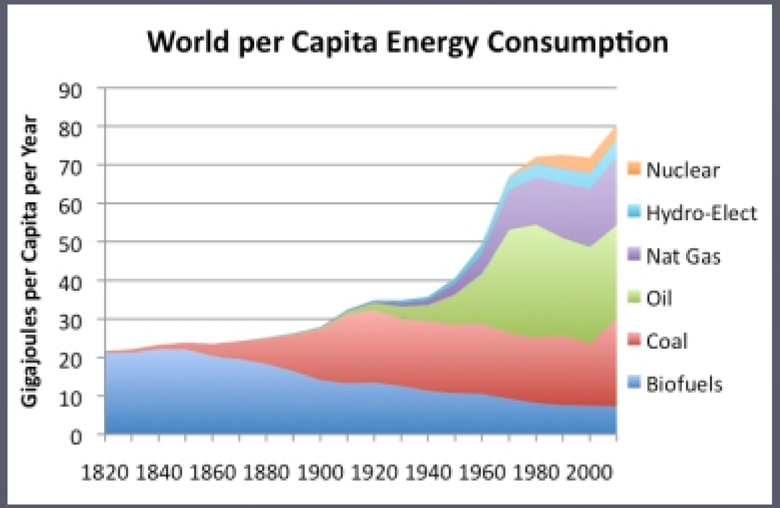
Fukushima Daiichi (2011)

Global Warming / Oil Spills

Tjernobyl (1986)

Deepwater Horizon (2010)

The Energy Problem



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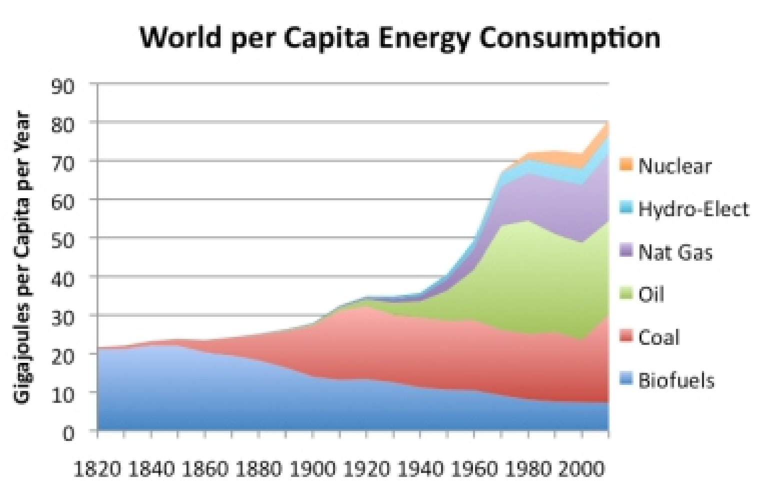
The most important scientific problem to solve for our modern society is how to convert and store clean energy.

The Energy Problem



Fukushima Daiichi (2011)

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The most important scientific problem to solve for our modern society is how to convert and store clean energy.

What is the Solution ???

Stationary Production

- Wind turbines

- Hydro-power

- Solar cells

- Geothermal

Mobile Production

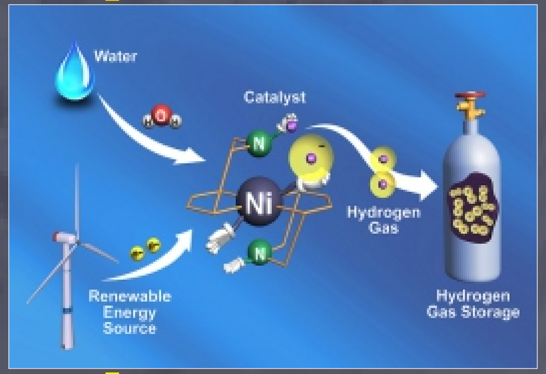
- Fuel cells

Energy Storage

- Batteries

- Hydrogen

Electrolysis



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Decentralized & fluctuating energy production

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Energy Storage

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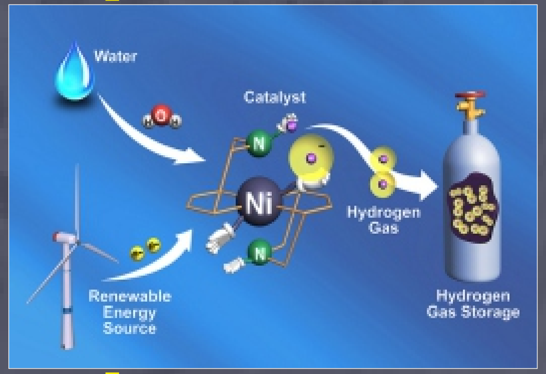
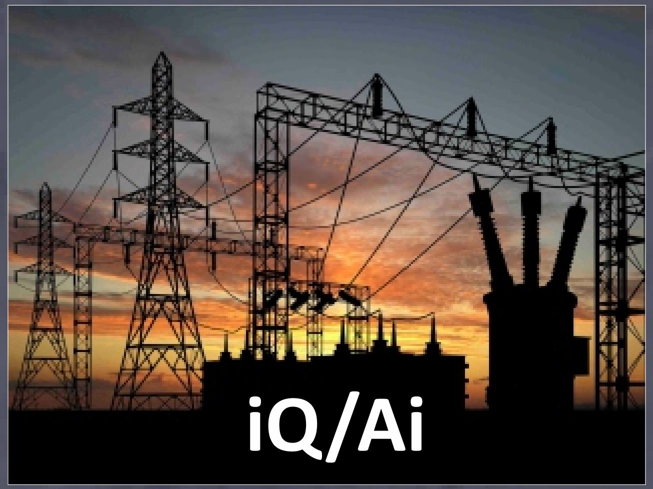


Smart Grids



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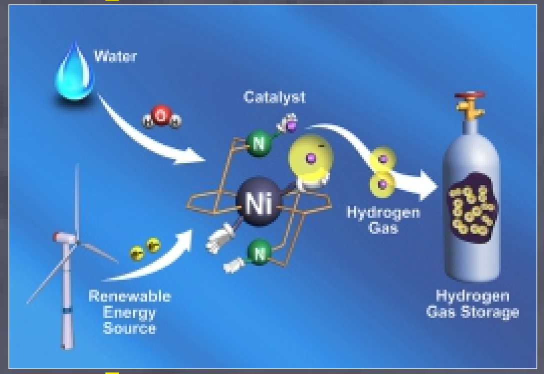

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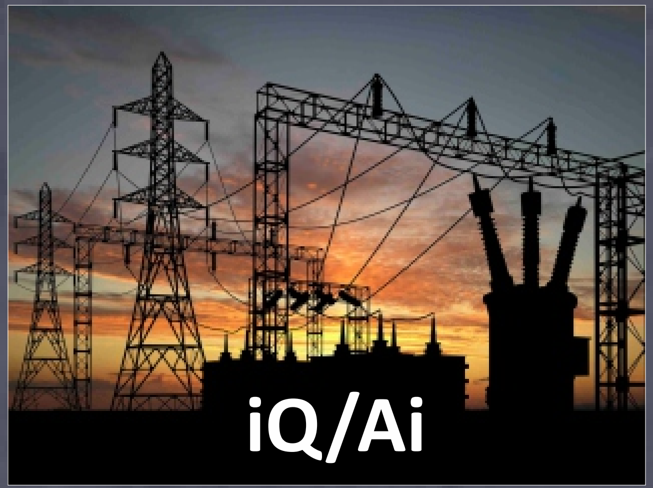
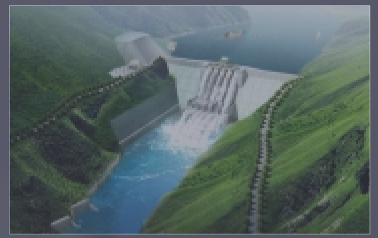


Decentralized & fluctuating energy production

Other alternative that we did not yet invent !!!

What is the Solution ??

Stationary Production

- Wind turbi
- Hydro-powe
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Decentralized & fluctuating energy production

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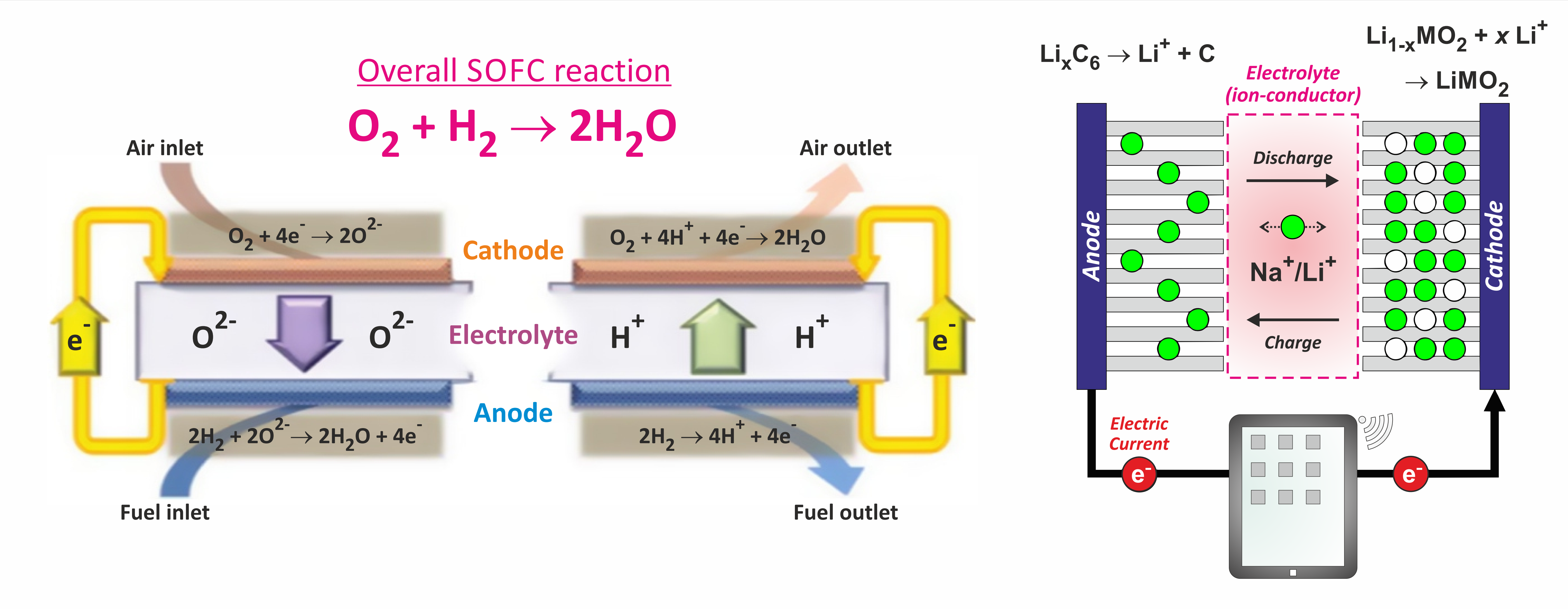
Electrolysis

Other alternative that we did not yet invent !!!

Energy Devices

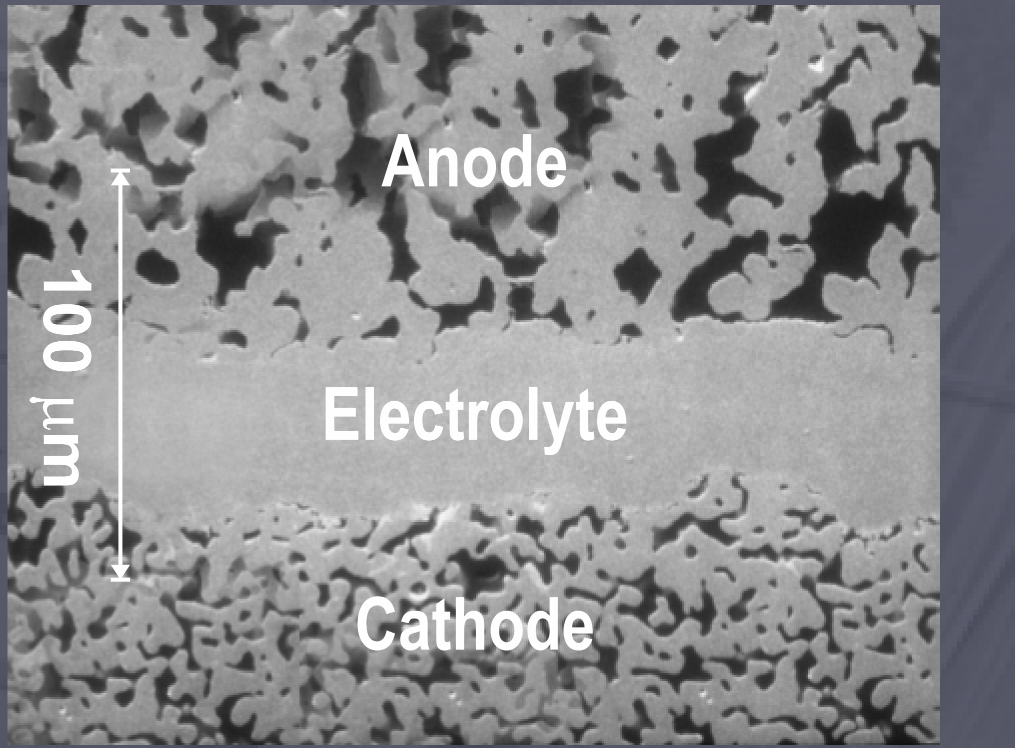
- Fuel cells as well as rechargeable batteries are electrochemical energy cells that directly transforms chemical energy into electricity.
- Very efficient devices: up to 85-98% efficiency !!! C.f. a normal combustion engine ~35-50%.



- Fuel cells use external fuel supply (*e.g.* H-storage) while batteries are chemically closed systems. + Fuel cells directly cause exhaust gases (H_2O, CO_2), while batteries only indirectly (power plant).

Solid State Fuel Cells & Batteries

- Solid-oxide fuel cells (SOFC) show highest efficiency but the *operating temperatures* should be lowered to 500-700°C to decrease cost while improving safety and lifetime.
- Main problem: Obtain high enough ionic conduction in solid state electrolytes + developing solid state H-storage.
- Present rechargeable batteries use electrolytes with organic solvents. Solid state batteries (SSB) are highly desirable from *safety* point of view but also for performance and lifetime. (Special case: Na-ion batteries!)



The key issue in future materials developments for SOFC & SSB is to understand ion diffusion mechanisms in the solid state on an atomic level, opening doors for tailored materials & improved device performance.

Hydrogen Storage

- Fuel cells are dependent on the supply of a fuel e.g. Hydrogen gas.
- Primitive form of hydrogen storage is simply a $H_2(g)$ bottle.

Overall SOFC reaction

$$O_2 + H_2 \rightarrow 2H_2O$$

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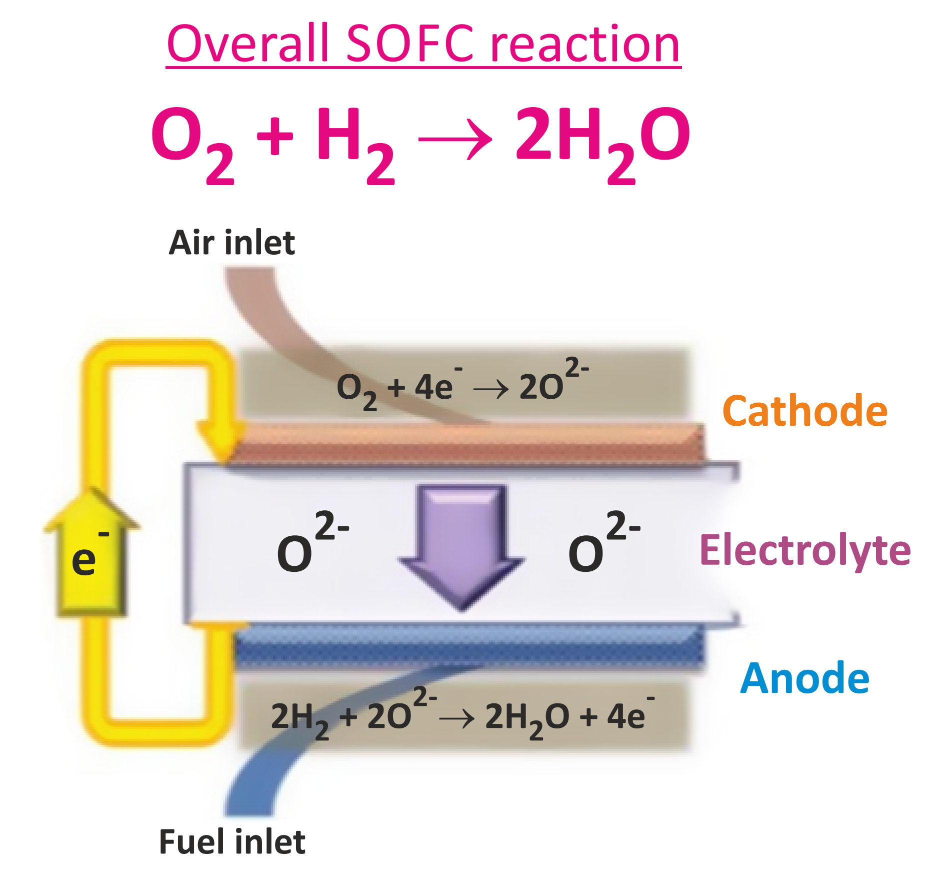
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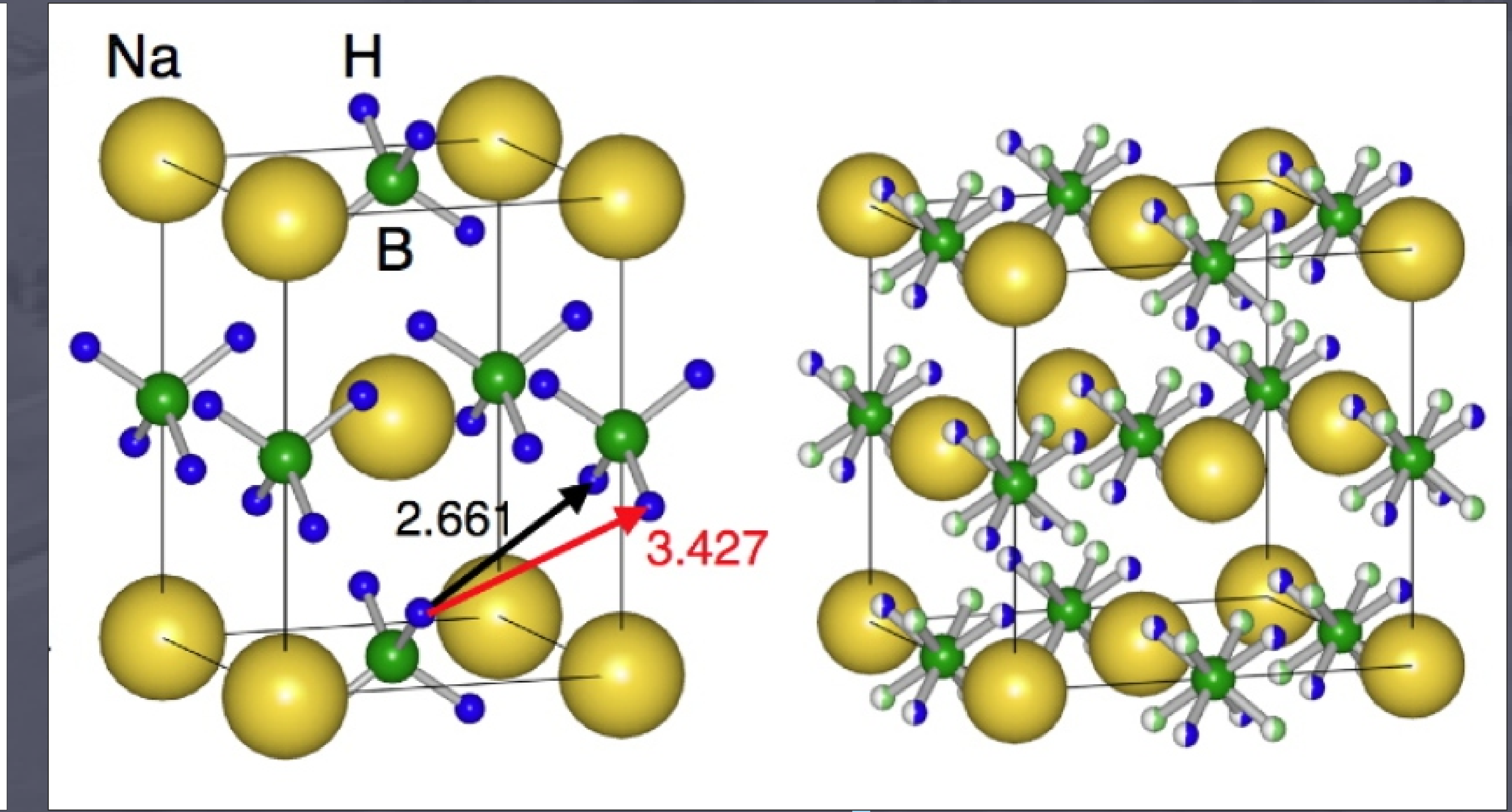
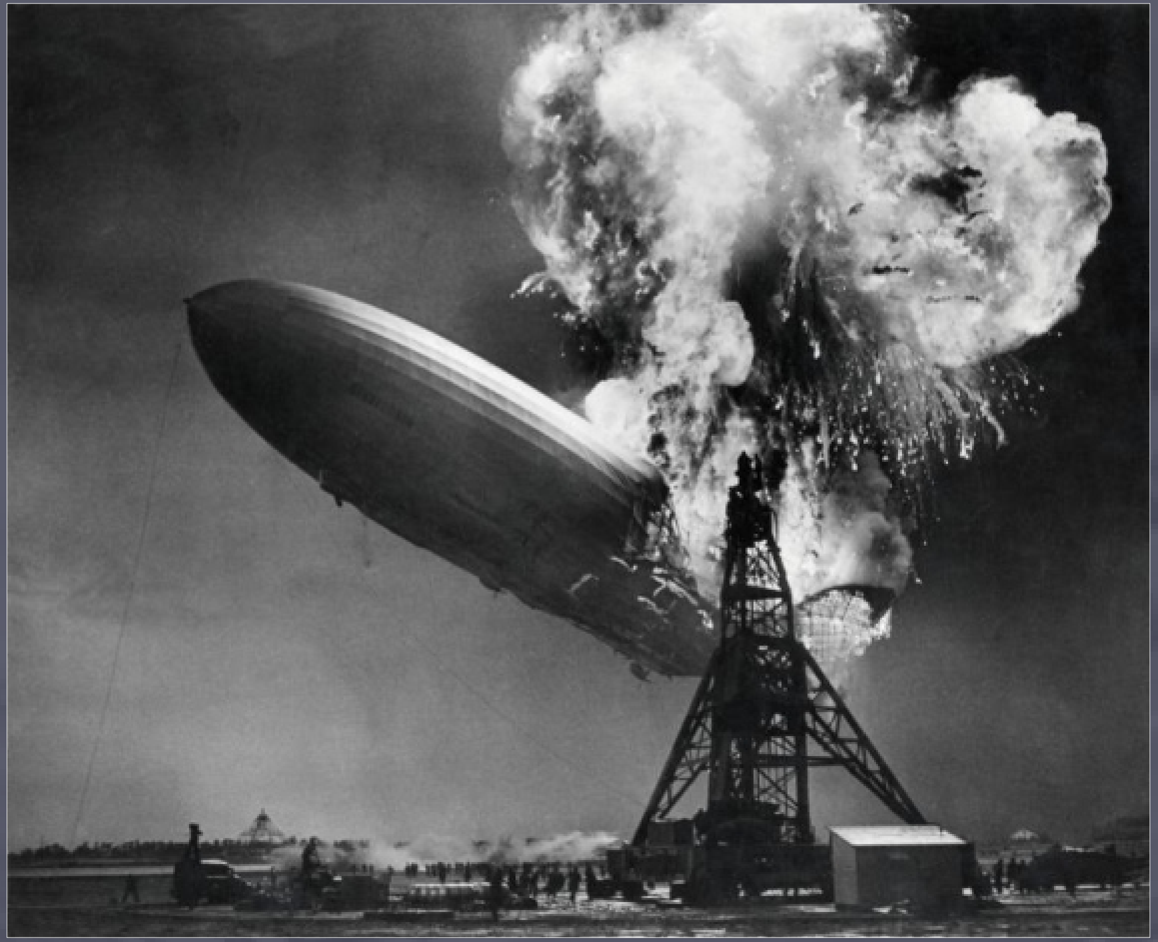


H_2(g)

- **However, also here the drive is for solid state devices i.e. solid state hydrogen storage, that has many advantages...**

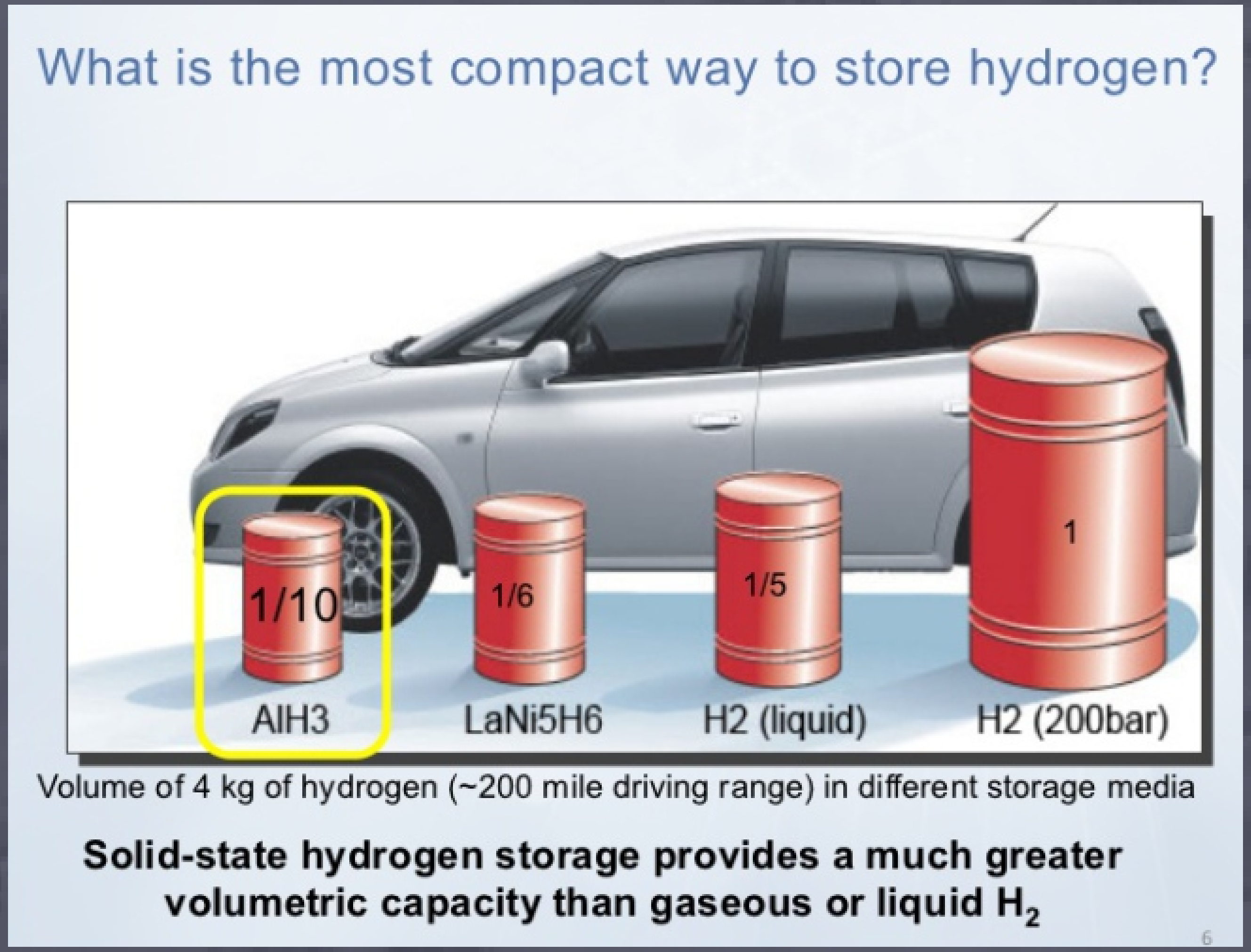
Benefits of Stolid-state H-storage

- Safety



<u>The Hindenburg Disaster</u>: Thursday, May 6, 1937, Lakehurst, New Jersey, United States

- Capacity

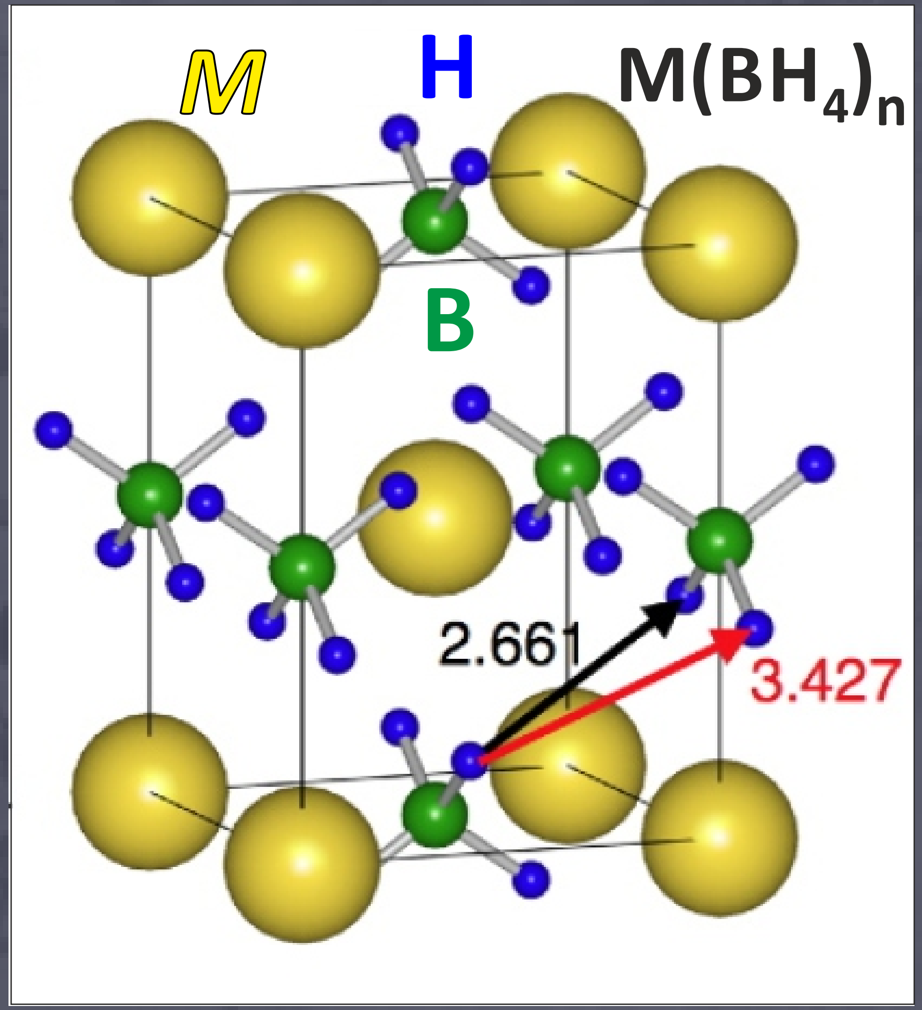


What is the most compact way to store hydrogen?

Volume of 4 kg of hydrogen (~200 mile driving range) in different storage media

Solid-state hydrogen storage provides a much greater volumetric capacity than gaseous or liquid H_2

- Complex Hydrides

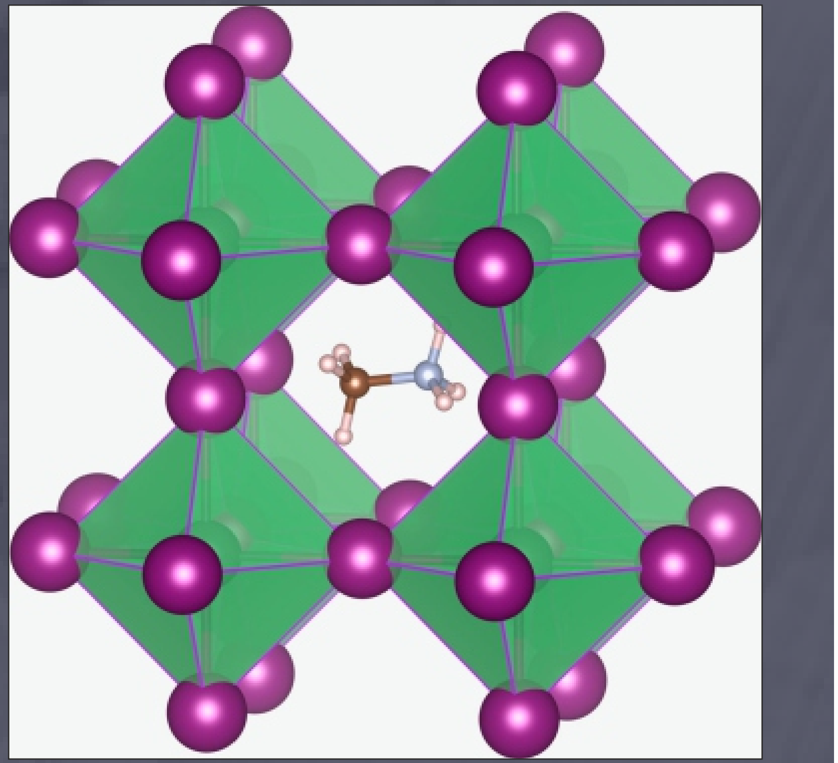


- Complex hydrides are heavily investigated as a H-storage material, particularly for cars
- Major problem is the high operating (desorption) temperatures
- Neutron scattering can uniquely study both H-structure and dynamics (diffraction, QENS, ...)

Photovoltaics / Solar Cells

- **The earth is a rather isolated place**
- **The only things we constantly receive is the 1 kW/m^2 of solar light.**
- **The sunlight striking earth's surface in 1h = energy to power the world economy for 1 year.**

- **This has made solar cells / photovoltaics one of the "hottest" research topics as well as business areas in the world.**
- **Main challenges involved first conversion efficiency but later also life-time/stability and production cost.**



- **There are many different kinds of techniques *e.g.* the hybrid perovskites, which is a class of organo-metallic lead / tin-halides**
- **There is a clear lack of fundamental understanding of electronic structures and lattice dynamics, which is needed for improving their performance.**

Future of Automobiles

"Past"

Combustion engine
100% fossil fuel (gasoline)
3.5 liter / 10 km

"Present"

Engine + El. motor
Gasoline + battery
0.3 liter / 10 km

"Future"

Electrical Motor
Fuel cell (H) + battery
0 liter / ∞ km

Main obstacles for the breakthrough of electric cars are cheap, safe and high-capacity batteries & H-storage !!!

Solid/Liquid Battery

Cathode ($LiCoO_2$)
Liquid Electrolyte + separator
Anode (Graphite)

All-solid-state Battery

Cathode ($LiFePO_4$)
Solid Electrolyte
Anode

Most Expensive Car-fire in the World

- Tesla Motor’s new Model S ($ 75'000 car)
- Caught fire on October 1:st, 2013 in Seattle USA

Reduced the value of Tesla Motor Company with $ 600 million !!!

This should be compared to the 180'000 combustion engine vehicles catching fire every year in USA !!!

Portable Electronics

- **Besides automotive applications the consumer electronics is the other large driving force for moving into solid state devices.**

Portable Electronics

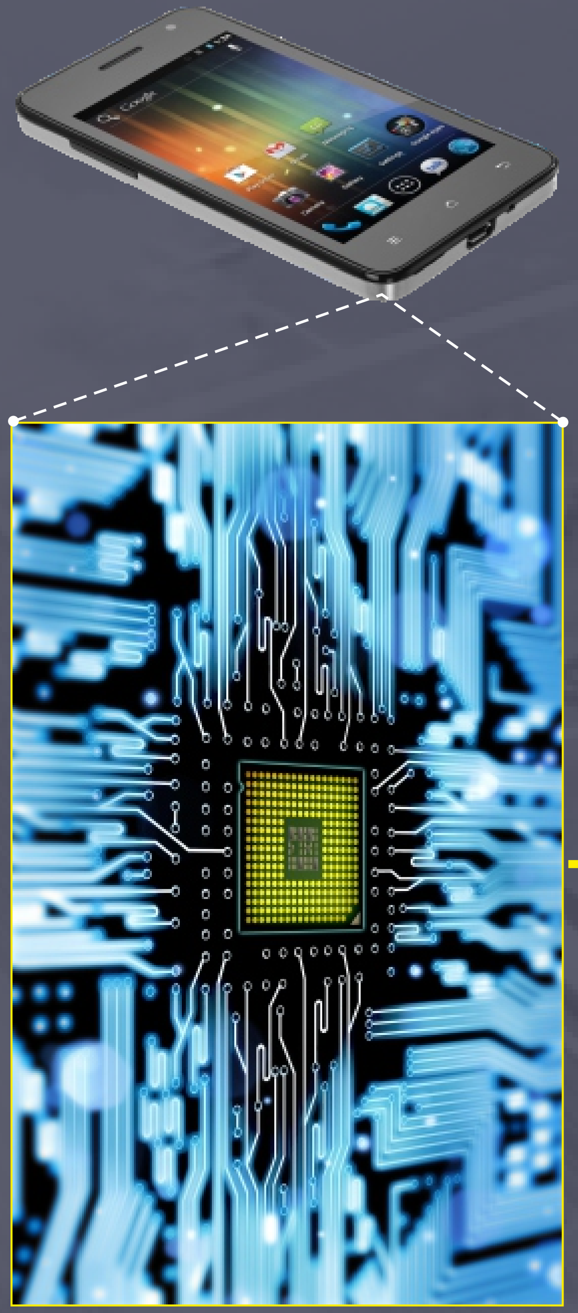
- Besides automotive applications the consumer electronics is the other large driving force for moving into solid state devices.

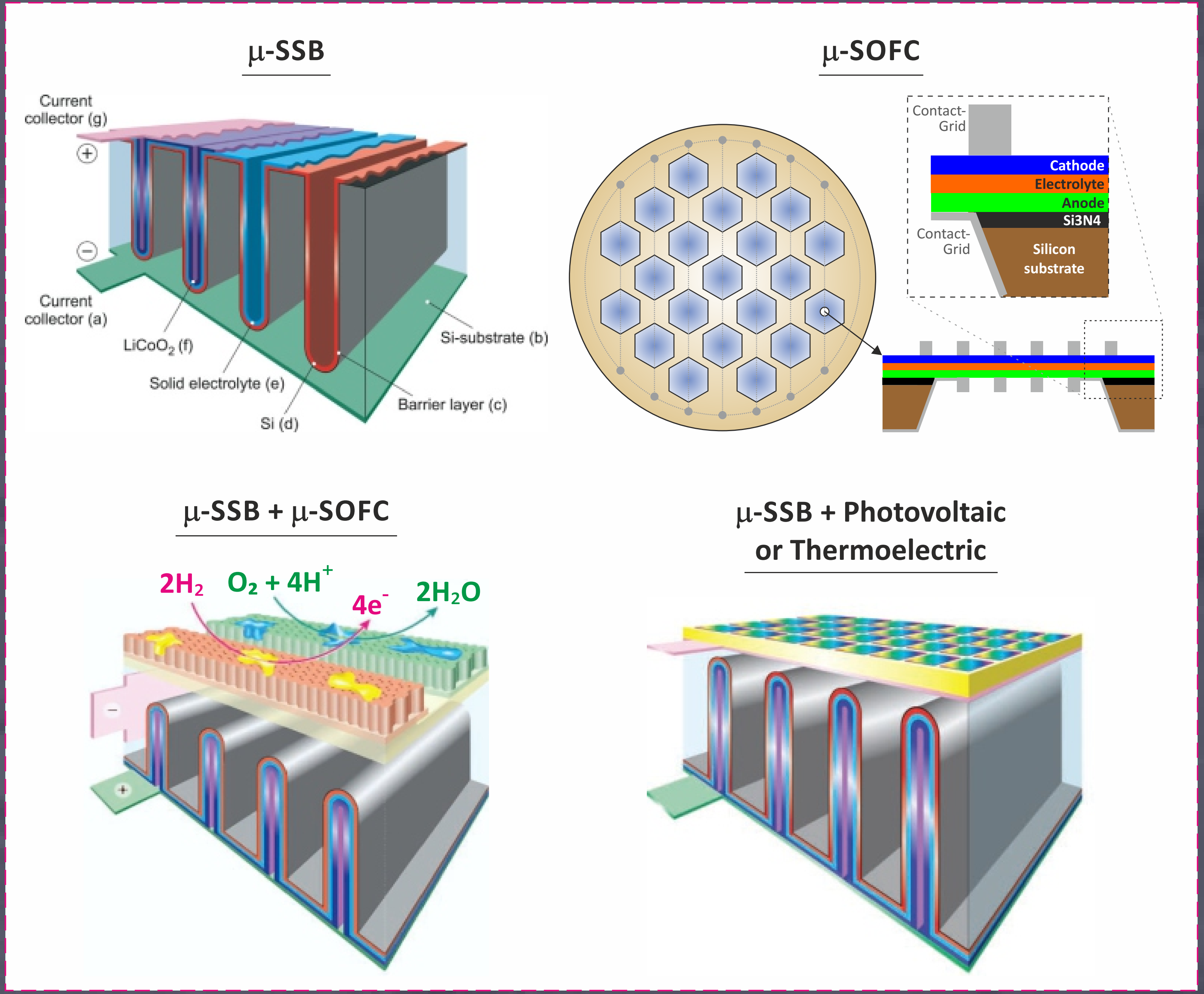
Where can I find a wall-socket to plug my smart-phone ?!?!?!

- These are the so-called **'wall-socket addicts'** that are frequently spotted at airports, trainstations & restaurants, scavenging the surroundings for power outlets to save their dying smartphone.

Energy Systems On-Chip (ESOC) Design

- Nano-scaling of materials show useful properties and new possibilities, *e.g.* higher ion diffusion rates and shorter charging times.



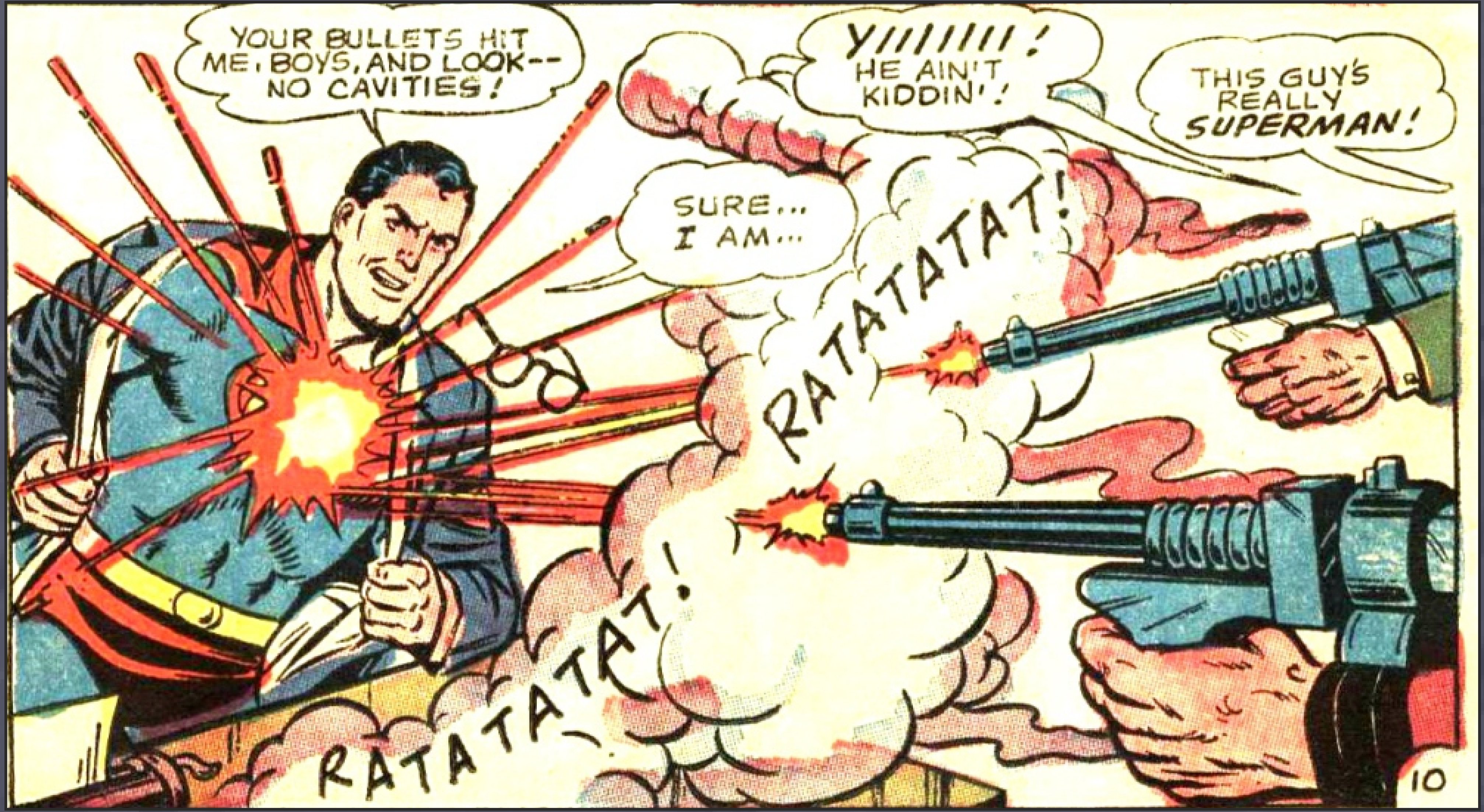


- Integrate energy systems in a similar way as other functions (SSD, wifi...) using an Energy Systems On-Chip (ESOC) design based on Si μ-fab.

- Unfortunately, solid state ionic transport is a very complex and poorly understood mechanism...

Solid State Ionics

- Transport of ions through a solid material, which is very difficult!



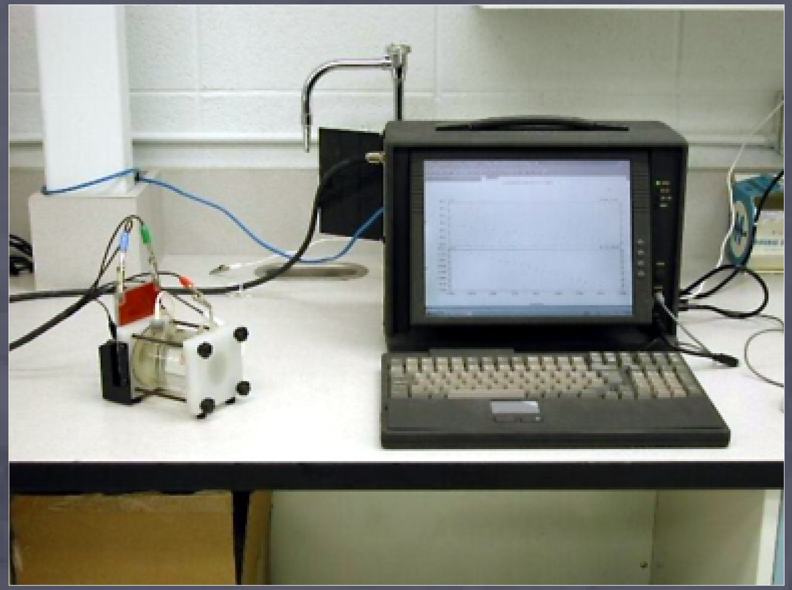
- Governed by very complex mechanisms (electronic, structural & strain fields) on an atomic level.
- The current understanding of such mechanisms is rather poor
- Main reason is the lack of suitable experimental methods that can efficiently study intrinsic material properties on an atomic scale.

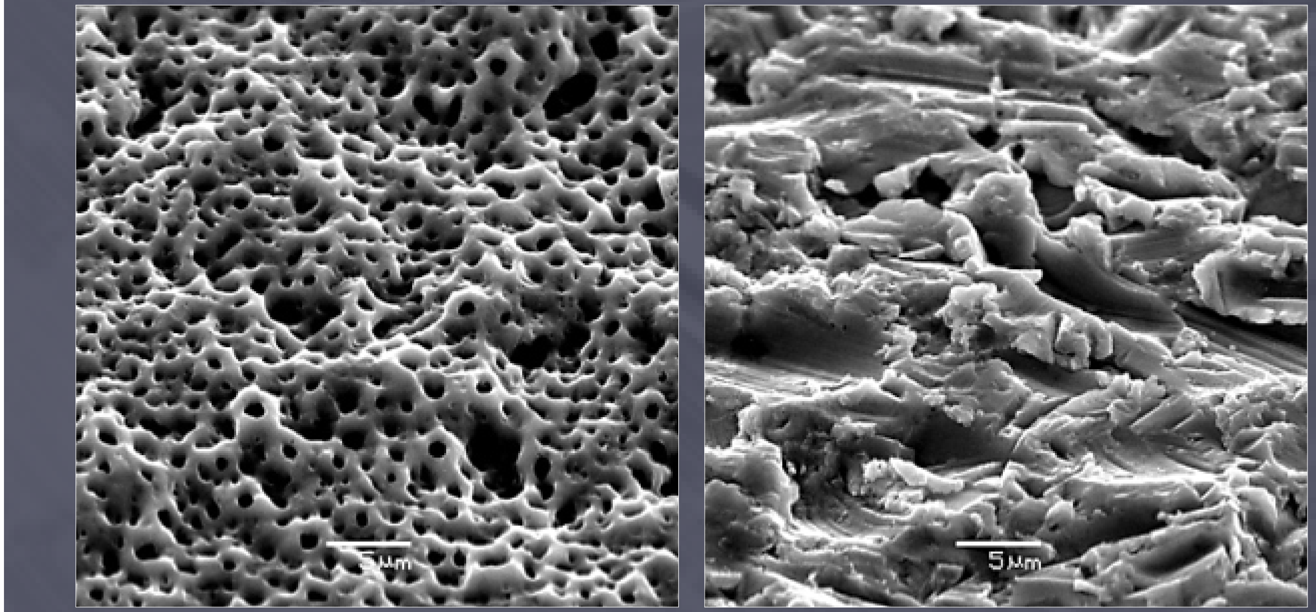
Electrochemical Methods

- The great success of current battery development have relied on electrochemical methods *e.g.*

  - *Electrochemical Impedance Spectroscopy* (EIS)
  - Galvanostaic Intermittent Titration Technique (GITT)
  - Potentiostatic Intermittent Titration Technique (PITT)

- These methods are quick, compact, relatively ’cheap’, and versatile... BUT they supply characterization of a complete device (or part of a) and NOT true intrinsic material properties.



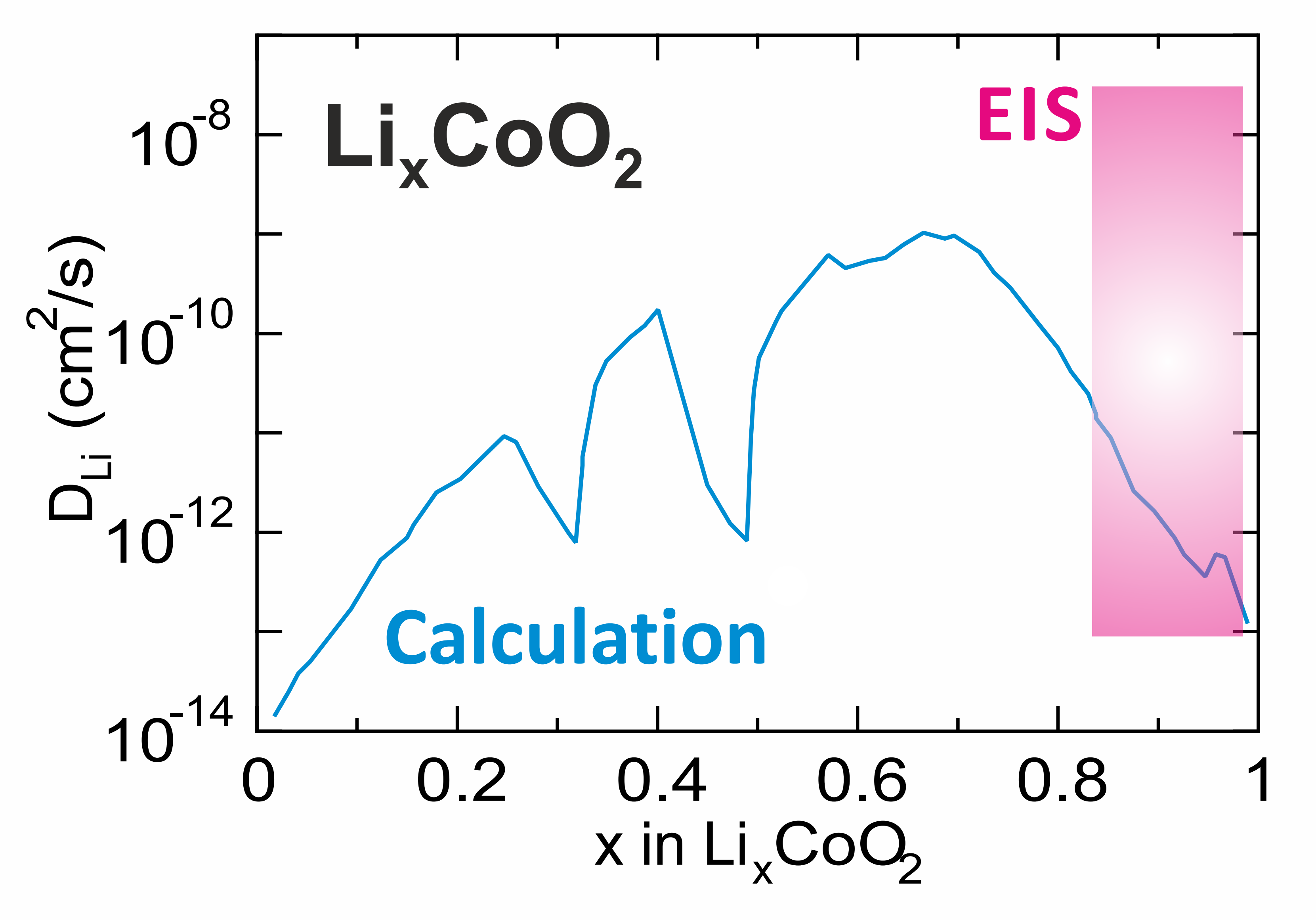


- Results obtained from electrochemical methods regarding *e.g.* the important ion diffusion coefficient D_{ion} are, hence, not only dependent on your material but also your device structure.

Electrochemical Methods

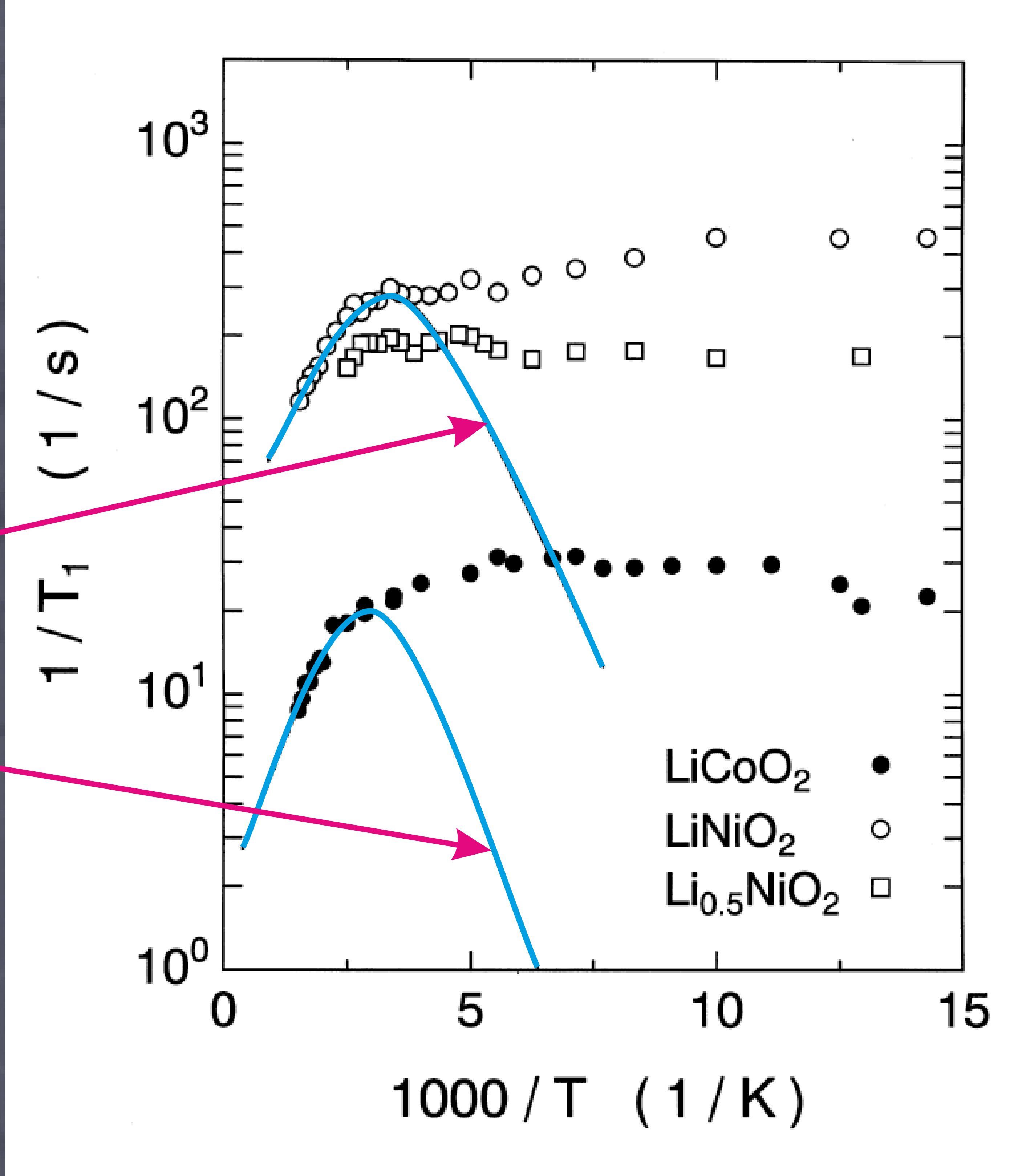
- As a result D_{ion} values are highly affected by how you build up your test cell, *e.g.*
  - Electrolyte composition
  - Microscopic structure (i.e. area) of the electrodes
  - How the individual device parts are affecting each other and/or interacting...
  - Surface and Interface effects

- The consequence is that absolute values of D_{ion} from electrochemical methods scatters over 5 orders of magnitude... from one and the same battery cathode material!



Nuclear Magnetic Resonance (NMR)

- Most important intrinsic material properties, D_{Li} , could not be measured accurately.
- Li-NMR is usually a good element selective method that yield intrinsic material properties.
- Magnetic ions induce additional relaxation pathways for spin-lattice relaxation ($1/T_1$), which do not follow theoretical predictions.
- D_{li} has instead been estimated from the NMR linewidth i.e. spin-spin relaxation ($1/T_2$), which is much more difficult.

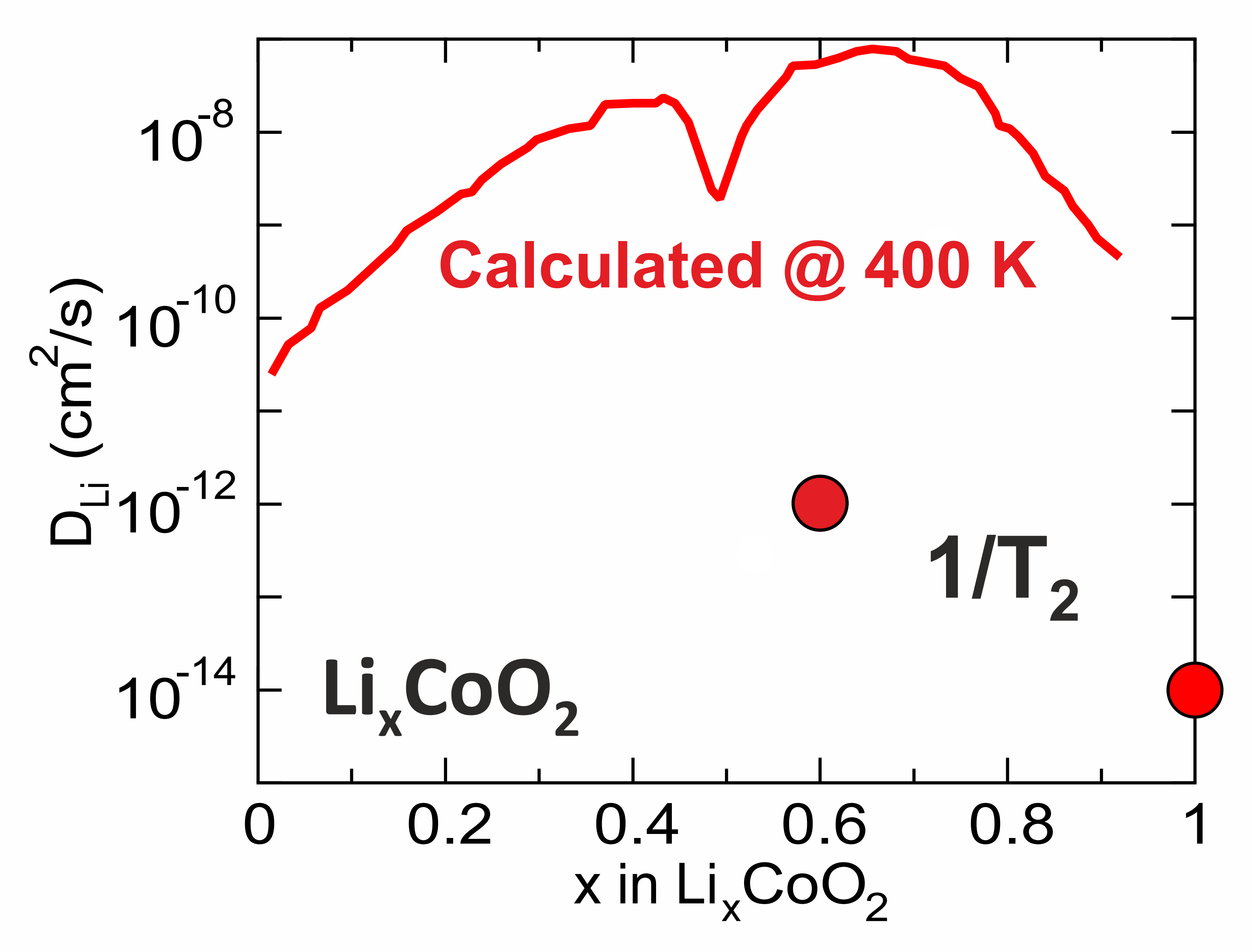


K. Nakamura *et al.*, Solid State Ionics 121, 301 (1999)

Nuclear Magnetic Resonance (NMR)

- **D_{li} is 5 orders of magnitude too small !!!** We can deduce what is moving but the absolute NMR numbers are unrnealistic:

- In order to take next step in this field we need to characterize solid state diffusion on the atomic level.



Van der Van, El. Chem. Sol. State Lett. 3, 301 (2000)

Make use of reliable microscopic methods i.e. state-of-the-art large-scale facilities.

Large-Scale Experimental Facilities

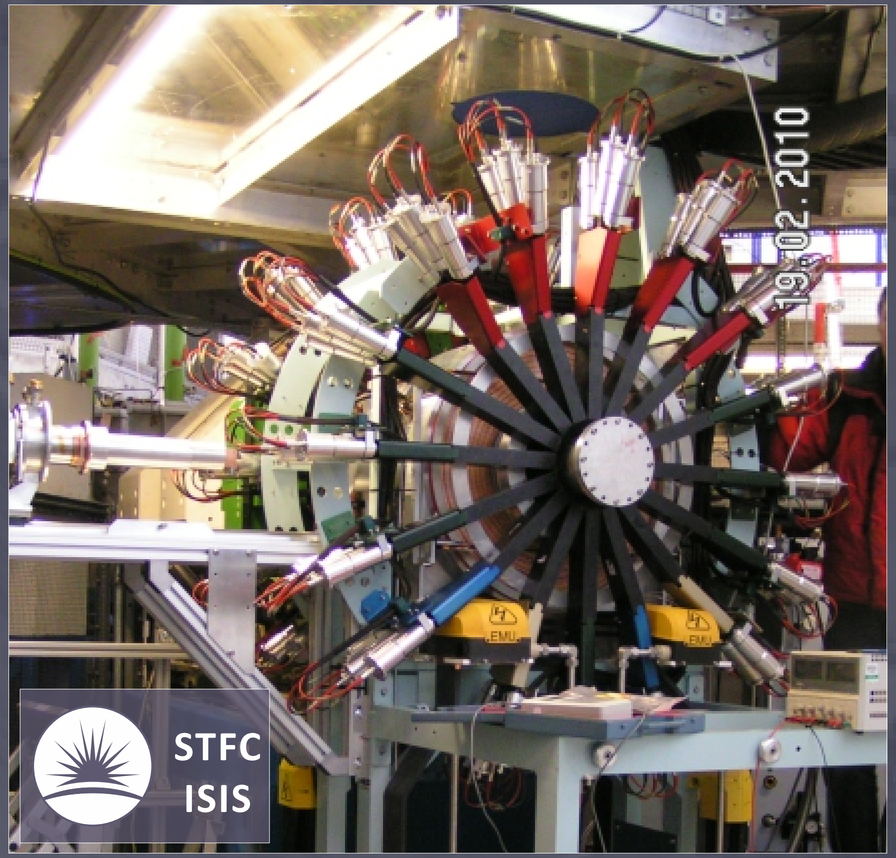
Synchrotrons

XRD, XAS, RIXS

Neutron Sources

NPD, SANS, QENS, IMAGING,
REFLECTOMETRY

Muon Facilities



ION-DIFFUSION, LEM

Free Electron Lasers

TIME-DEPENDENCE, BRILLIANCE

Large-Scale Experimental Facilities

Synchrotrons

XRD, XAS, RIXS

Neutron Sources

NPD, SANS, QENS, IMAGING, REFLECTOMETRY

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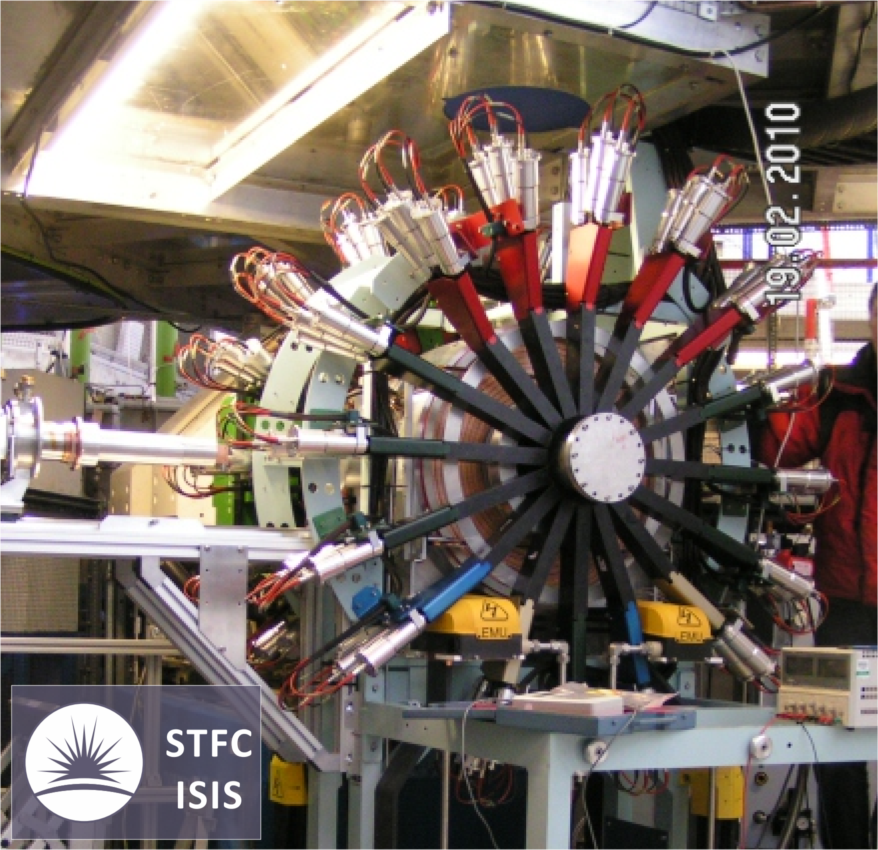


Free Electron Lasers

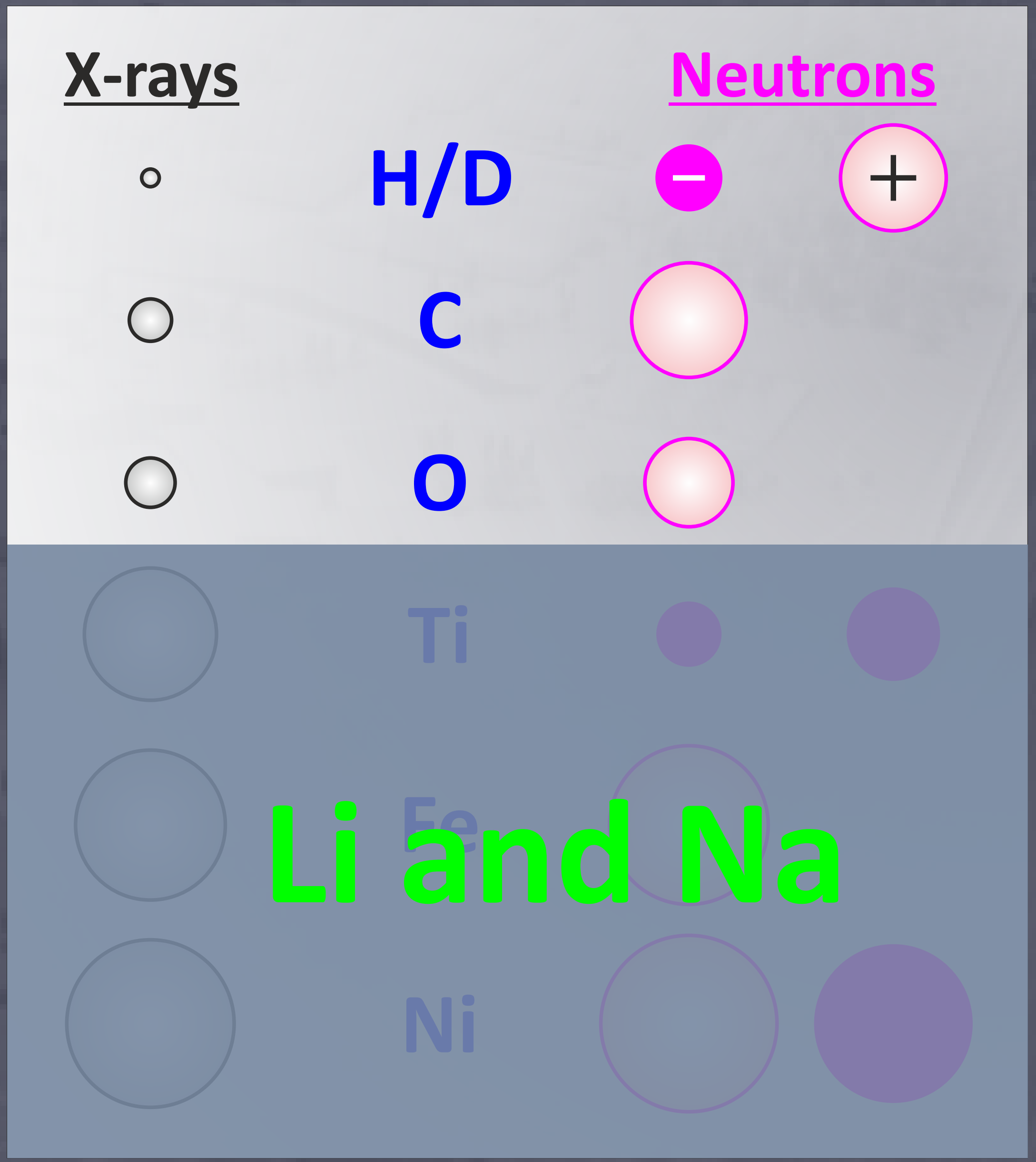
TIME-DEPENDENCE, BRILLIANCE

Why Neutrons for Energy Materials?

Why Neutrons for Energy Materials?

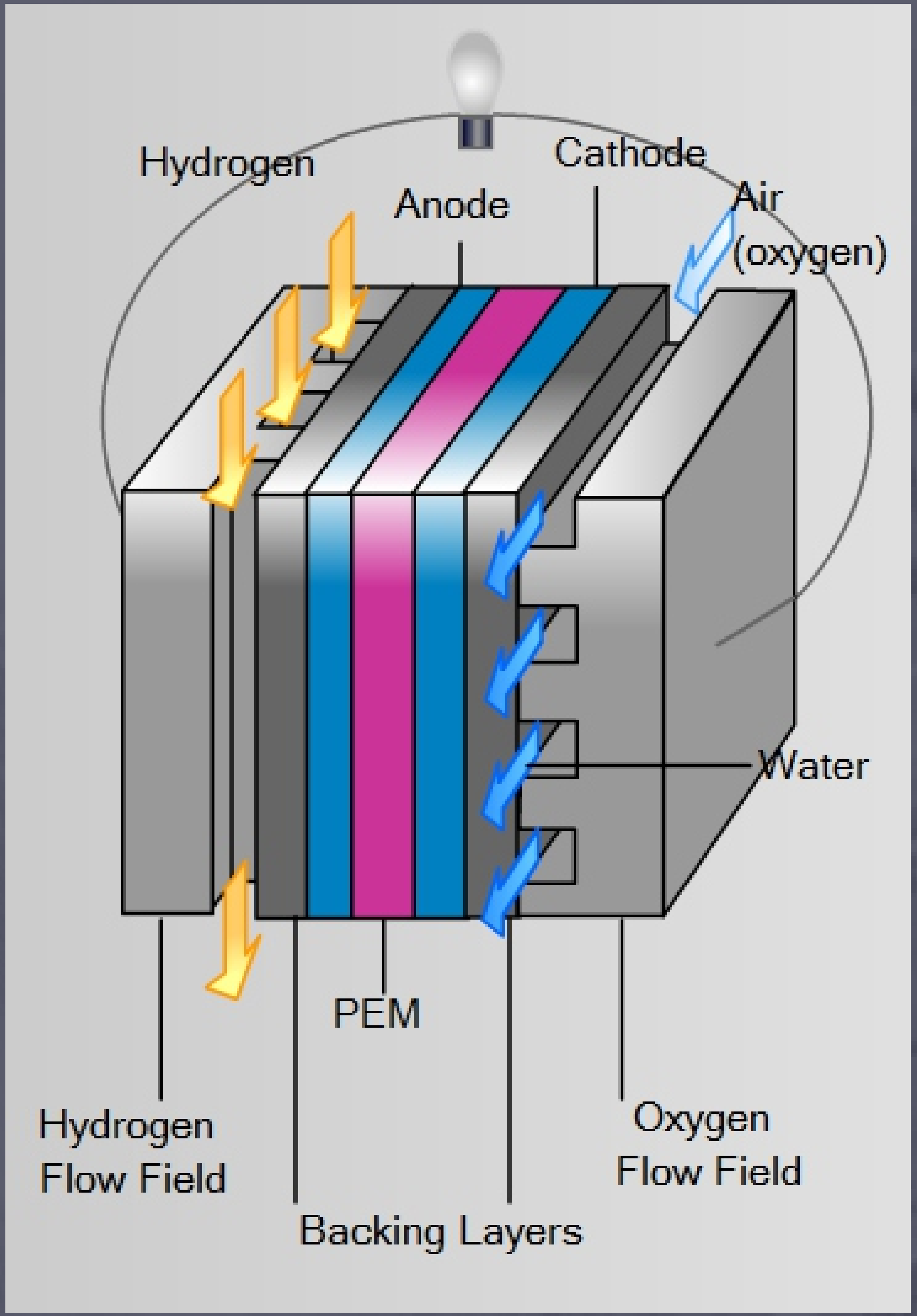
- Neutron wavelengths/energies are perfect for studying material properties on an atomic scale.
- Point-interaction with nuclei (not only e^-) → can study structure of light elements + Q-independent form-factor (c.f. x-rays!).
- Inelastic experiments allow to study dynamics of atoms/ions.
- Strong nuclear and magnetic scattering.
- Isotopic sensitivity → contrast variation e.g. H/D with -/+ scattering lengths i.e. 180° out of phase !!!
- Penetrating: probe bulk properties & buried structures making it possible to perform *in situ* or even *in operando* measurements.
- Measurements under extreme conditions: low (T = 10 mK) and high (1500 K) temperatures, high pressures (P = 100 kbar) and magnetic fields (H = 20 T).

Scattering Strengths



Neutrons can tell us where atoms are and how spins align... but also what they do!

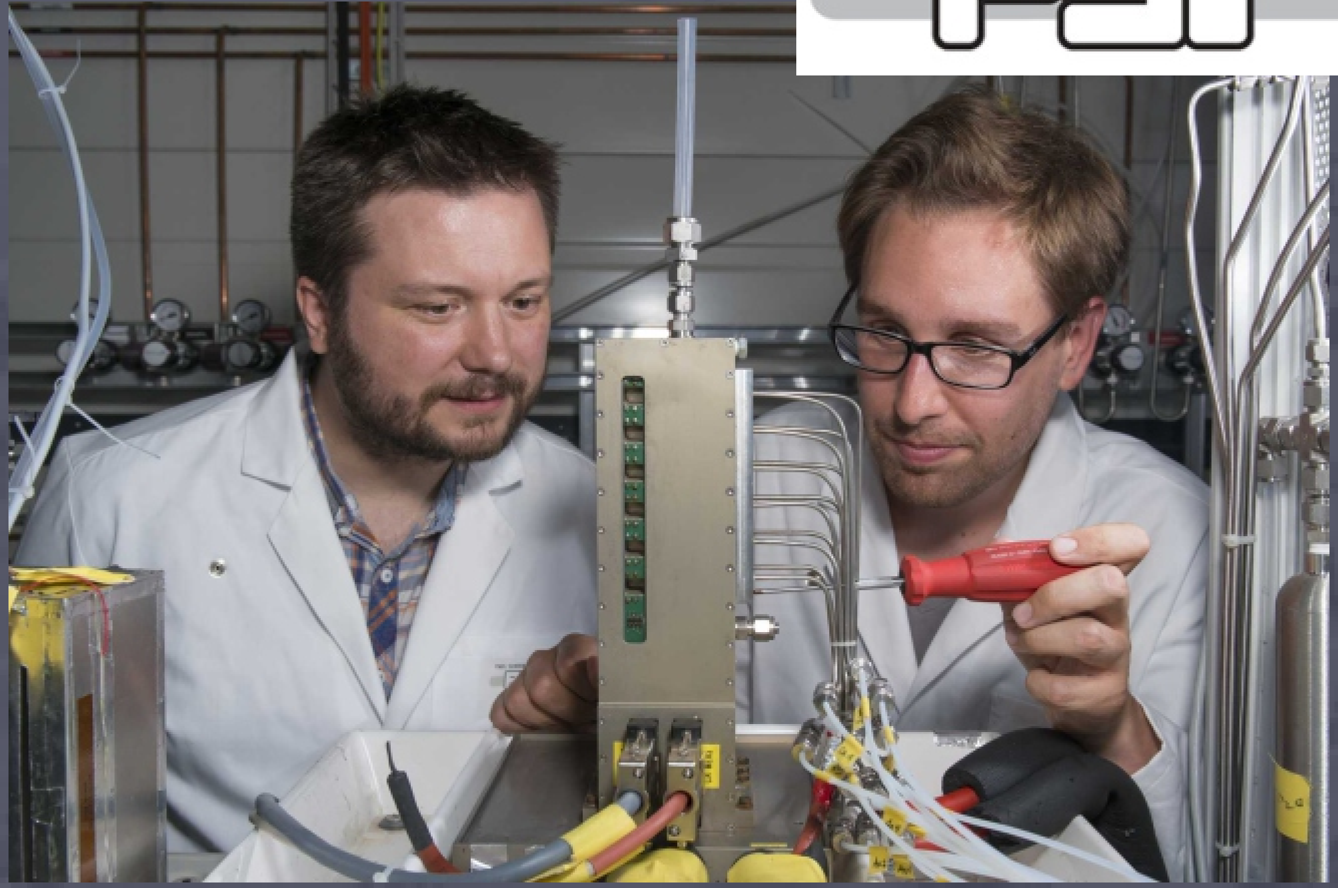
Ex. #1: Neutron Imaging: Fuel Cells

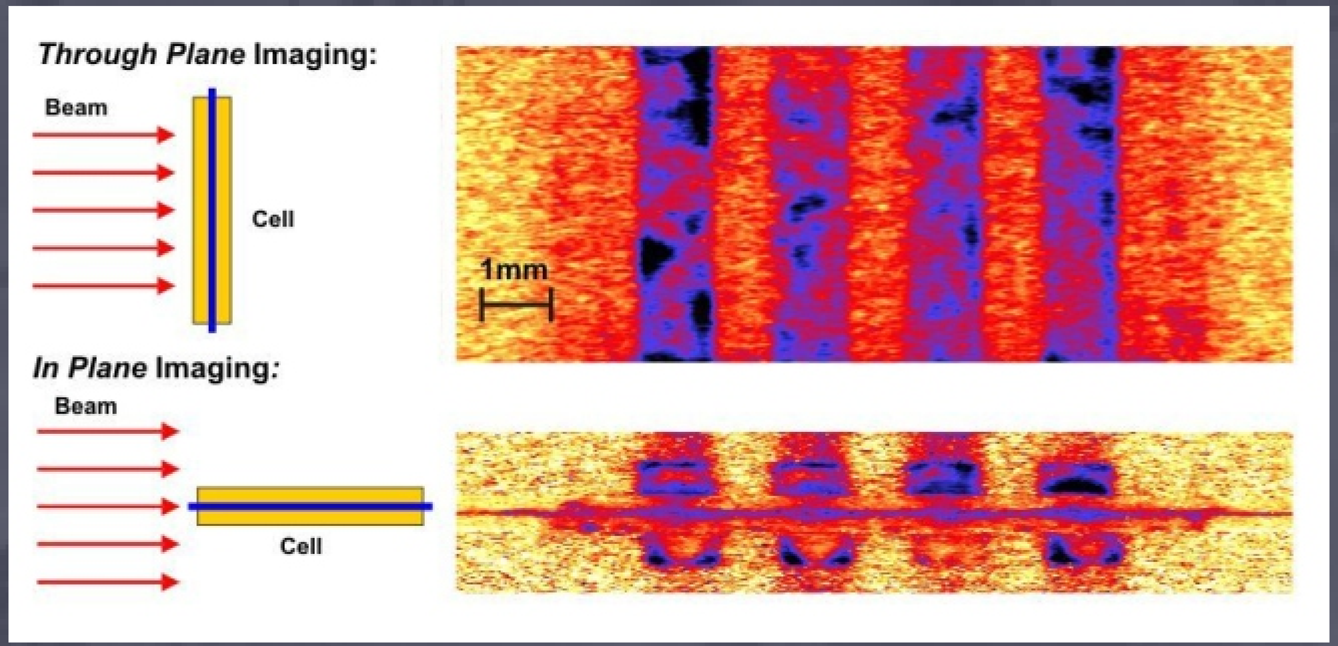


H_2O

PAUL SCHERRER INSTITUT

PSI



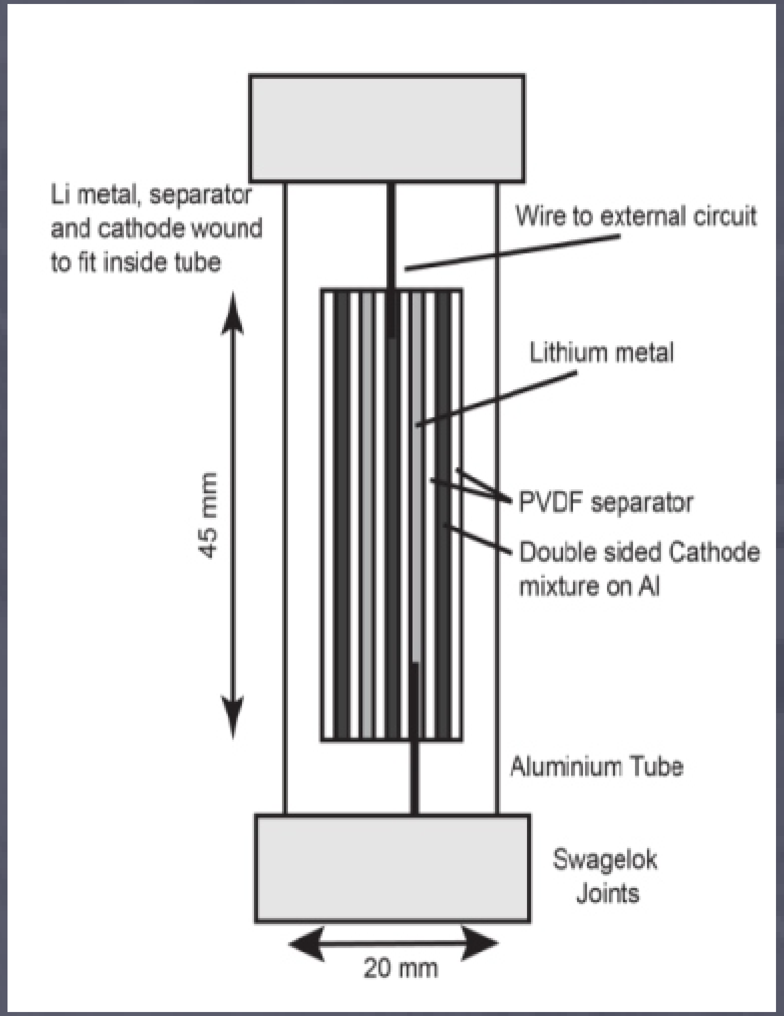


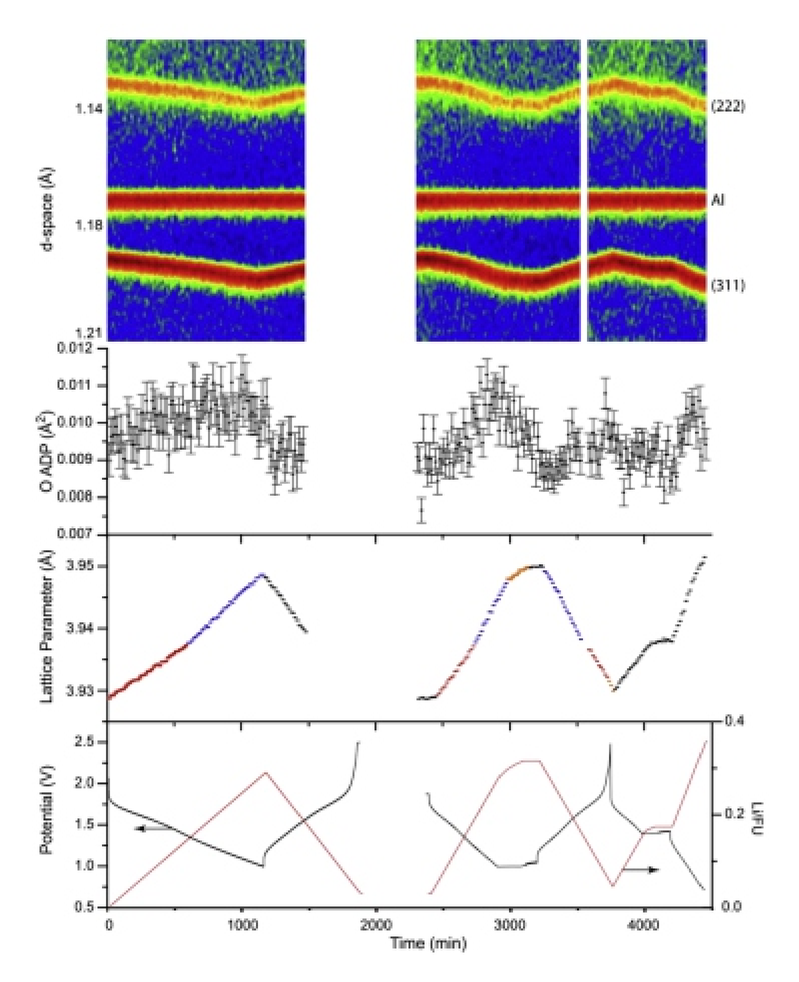
Already covered
in lecture by
Prof. L. Theil Kuhn !!!

Batteries: in operando neutron diffraction

- **Understanding changes in the atomic structure of the electrode materials in re-chargeable batteries as a function of charge/dis-charge cycles is a key aspect to improve their lifetime.**
- **There are many many groups working in this field around the world and there are many different set-ups for performing such measurements.**
- **One “type” is the design of special battery cells that are meant to “mimic” a real battery cell while still being “optimized” for neutron scattering.**

W.R. Brant et al., J. Power Sources 336, 279 (2016)



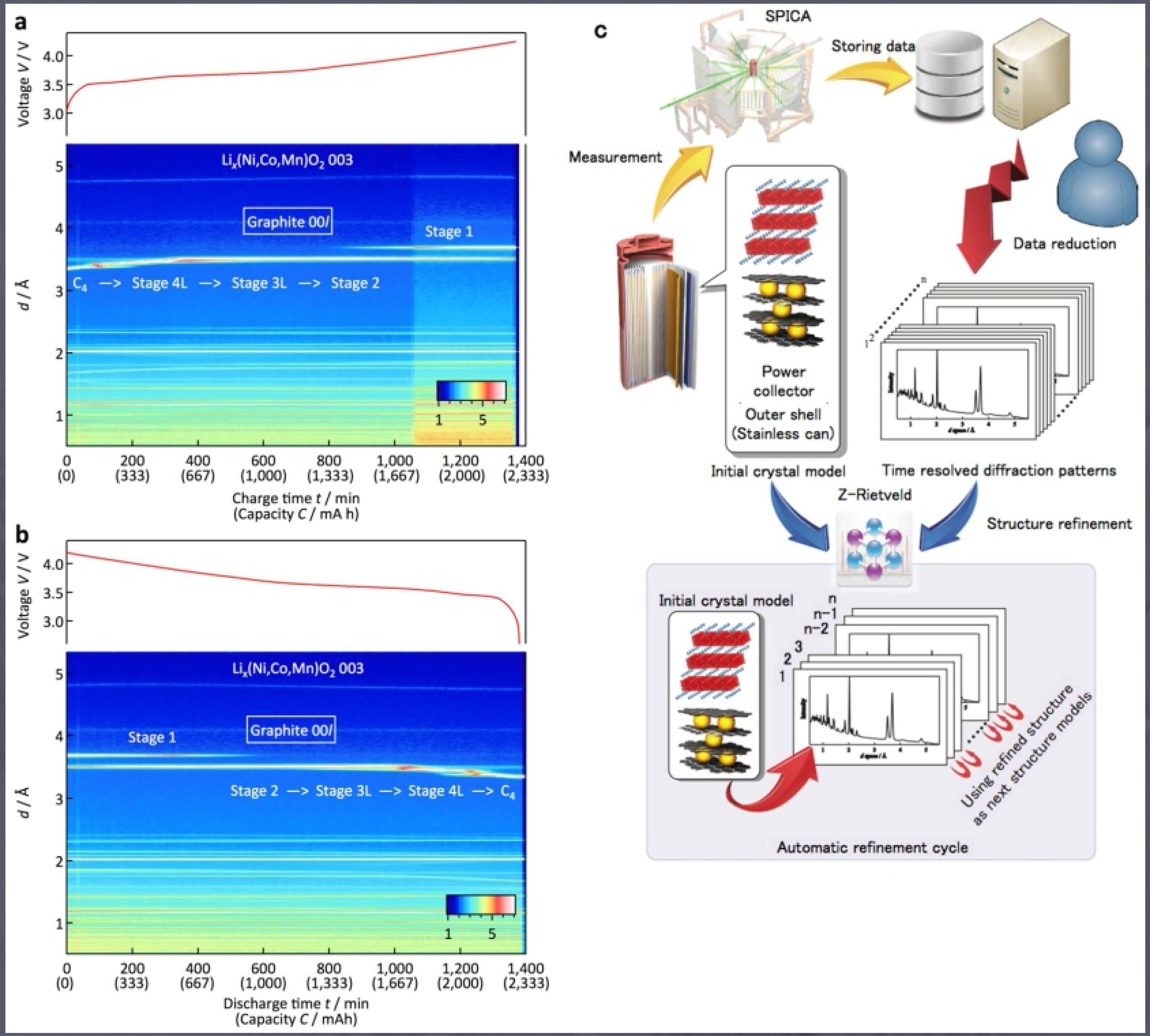


- **With such cells it is possible to directly follow the atomic structure during cycling (*in operando*).**
- **One successful project at Uppsala University...**
- **But there are similar ones at e.g. PSI, SNS and J-PARC.**

Batteries: “Commercial” in operando

- The other “school” within this competitive field is the groups looking directly at commercial batteries directly in the neutron beam.

S. Taminato et al., Scientific Reports 6, 28843 (2016)

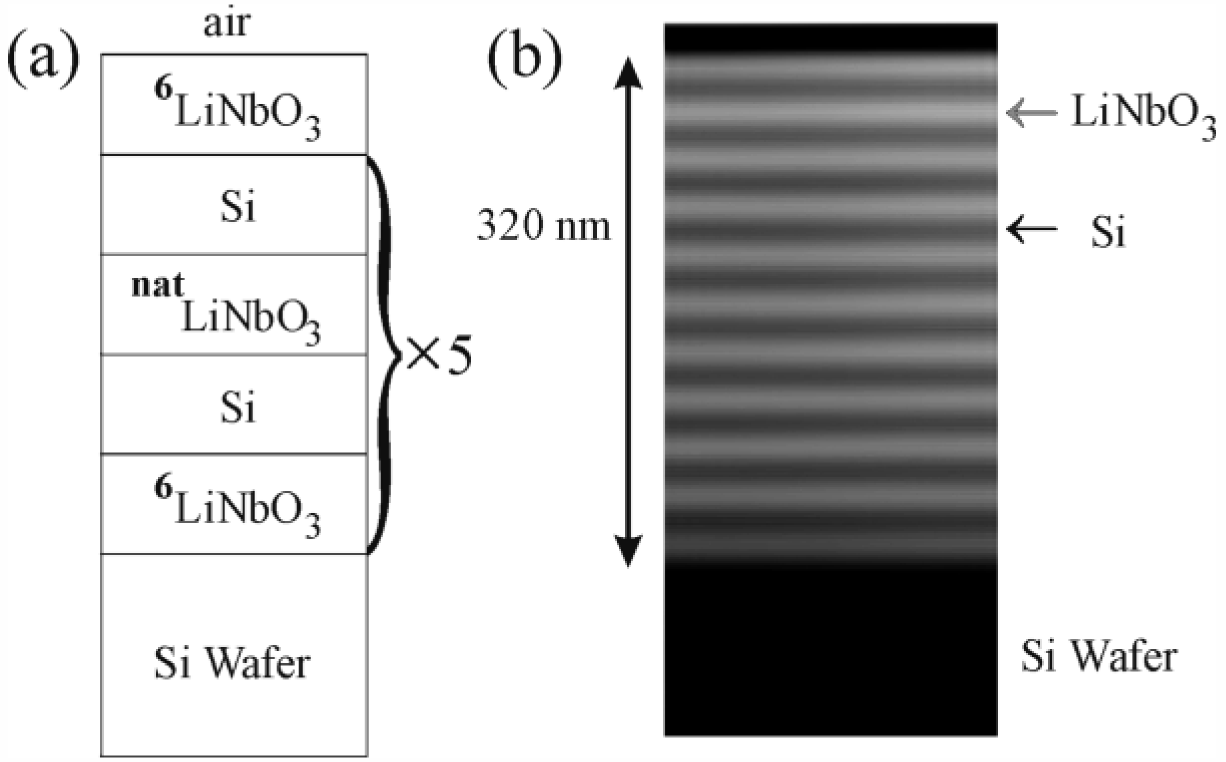


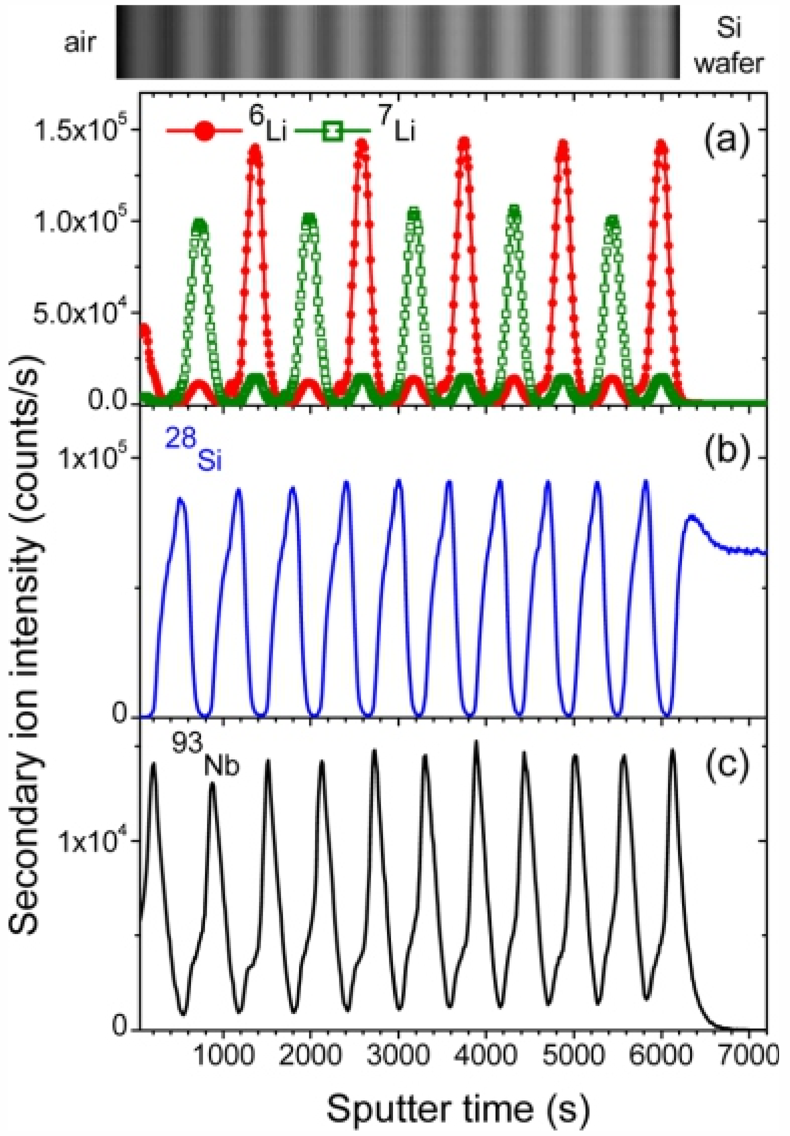
- This example comes from J-PARC where the experimental system comprising a time-of-flight diffractometer with automated Rietveld analysis.
- The setup collects and analyze diffraction data produced by sequential charge/discharge processes.
- More industrial approach giving huge collection of data sets.
- Complex understanding of how material properties & engineering are linked in a device.

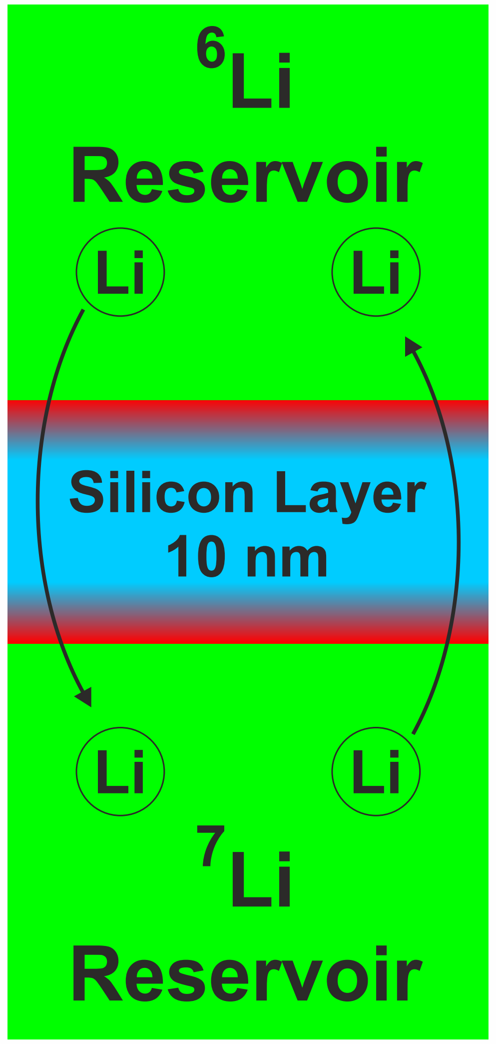
Ion Diffusion by Neutron Reflectometry

- Neutron reflectometry (NR) is the neutron technique ideal for looking at thin-film energy materials *e.g.* solid state battery structures.
- Multilayer structure of alternating $LiNbO_3$ and thin amorphous Si layer.
- By clever growth using alternating ^{6}Li and ^{7}Li isotopes it is possible to use contrast difference to study ion diffusion through the Si layer by NR.

Erwin Hüger *et al.*
Clausthal University of Technology
Germany





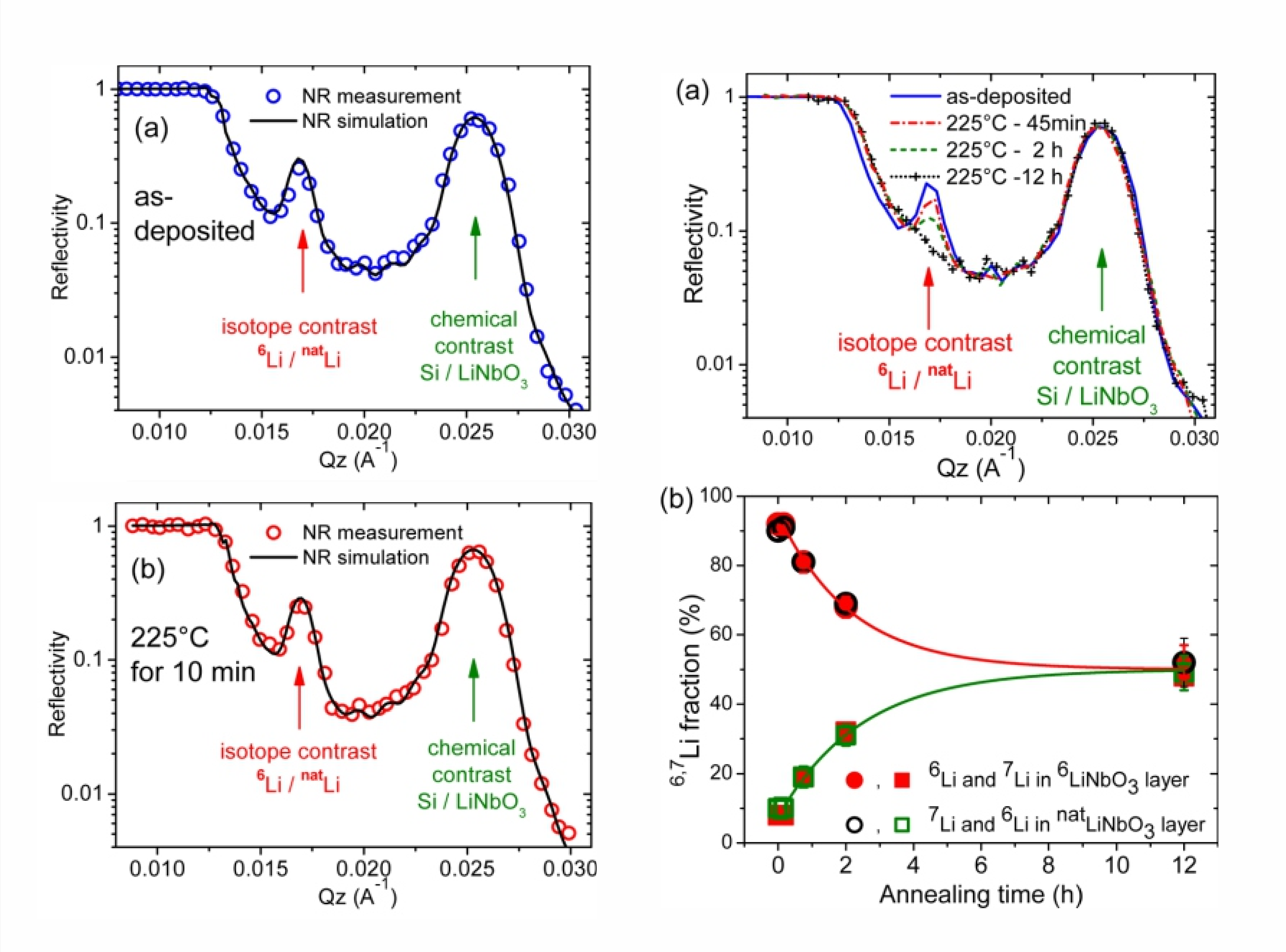


Ion Diffusion by Neutron Reflectometry

- By collecting NR data as a function of time for elevated temperature it is possible to follow how Li-ions diffuse across the Si layer.
- By modelling it is then possible to extract the Li-ion diffusivity:

$$D_S \approx 6 \times 10^{-13}\ \mathrm{cm^2/s}$$

- Similar studies have also been performed for films on single crystals, which gives the self Li-ion diffusion in $LiNbO_3$.
- Interesting tool for studying ion diffusion in thin films with influence from strain effects as well as interface issues...



E. Hüger *et al.*

- Adv. Engineering Materials 11, 446 (2009)
- Nano Letters 13, 1237 (2013)
- Phys. Chem. Chem. Phys. 16, 3670 (2014)

Ion Diffusion by Neutron Reflectometry

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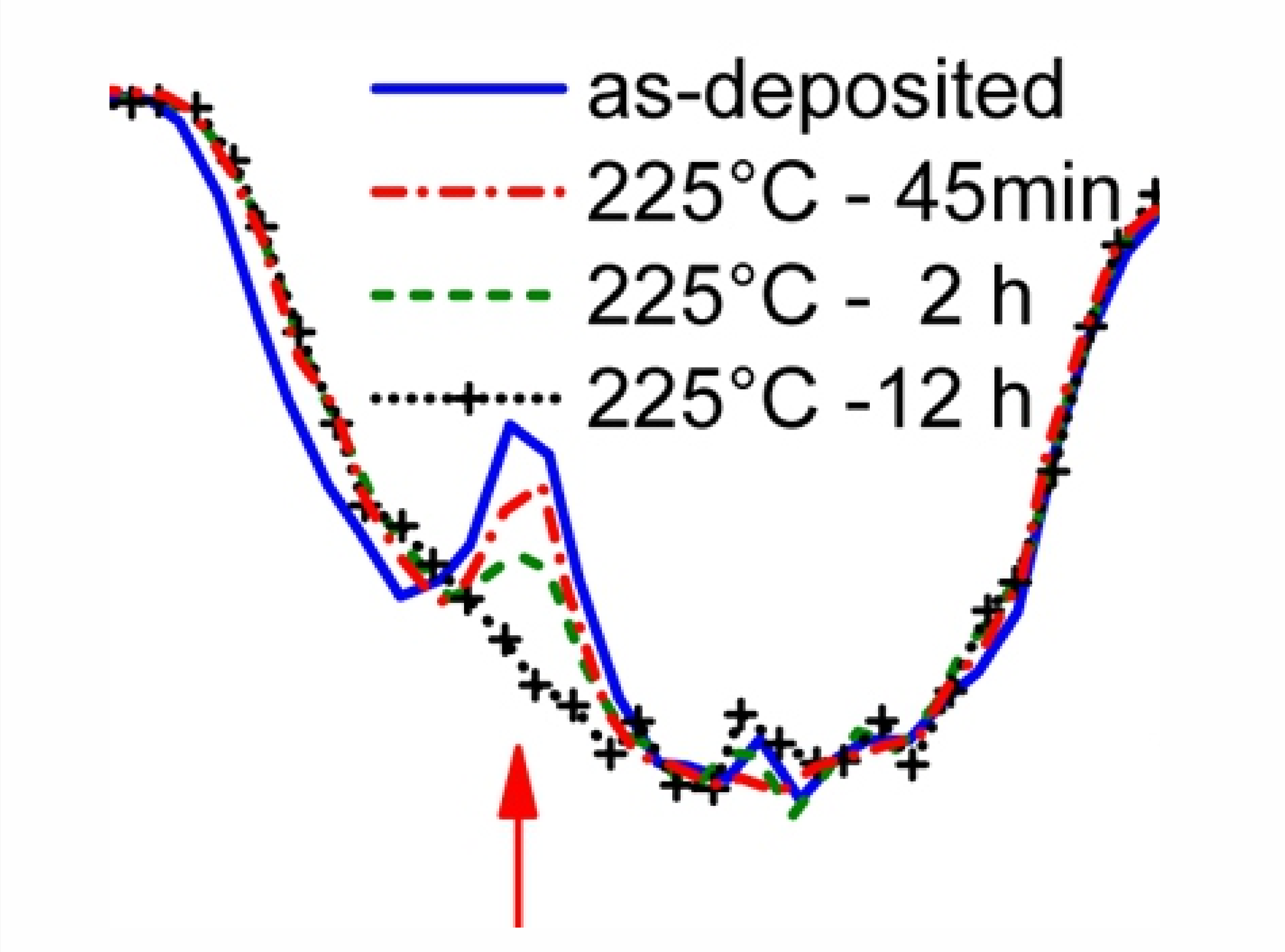
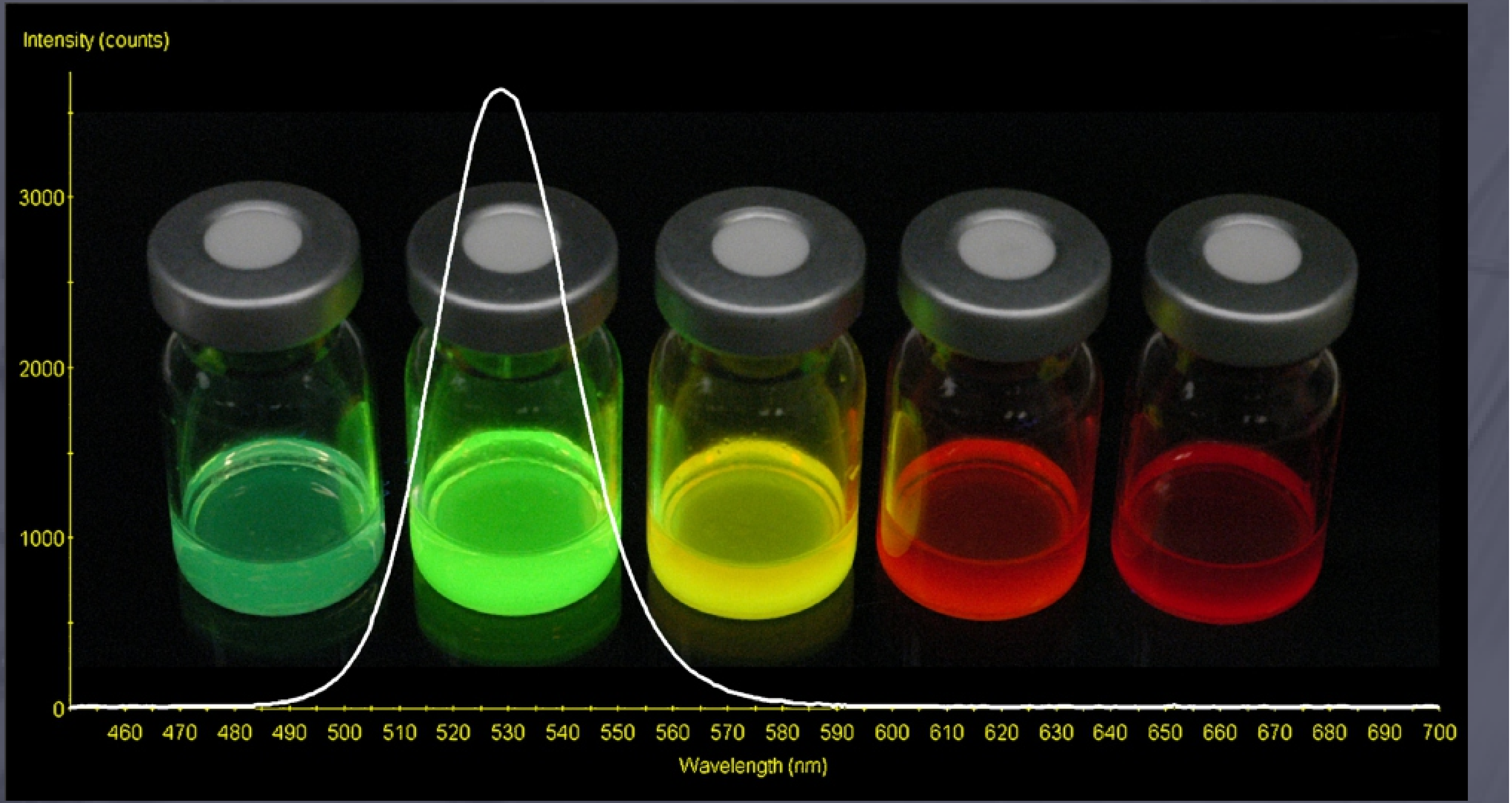


E. Hüger *et al.*
- Adv. Engineering Materials 11, 446 (2009)
- Nano Letters 13, 1237 (2013)
- Phys. Chem. Chem. Phys. 16, 3670 (2014)

Short Coffee Break !!!

Nano-structured PV Materials

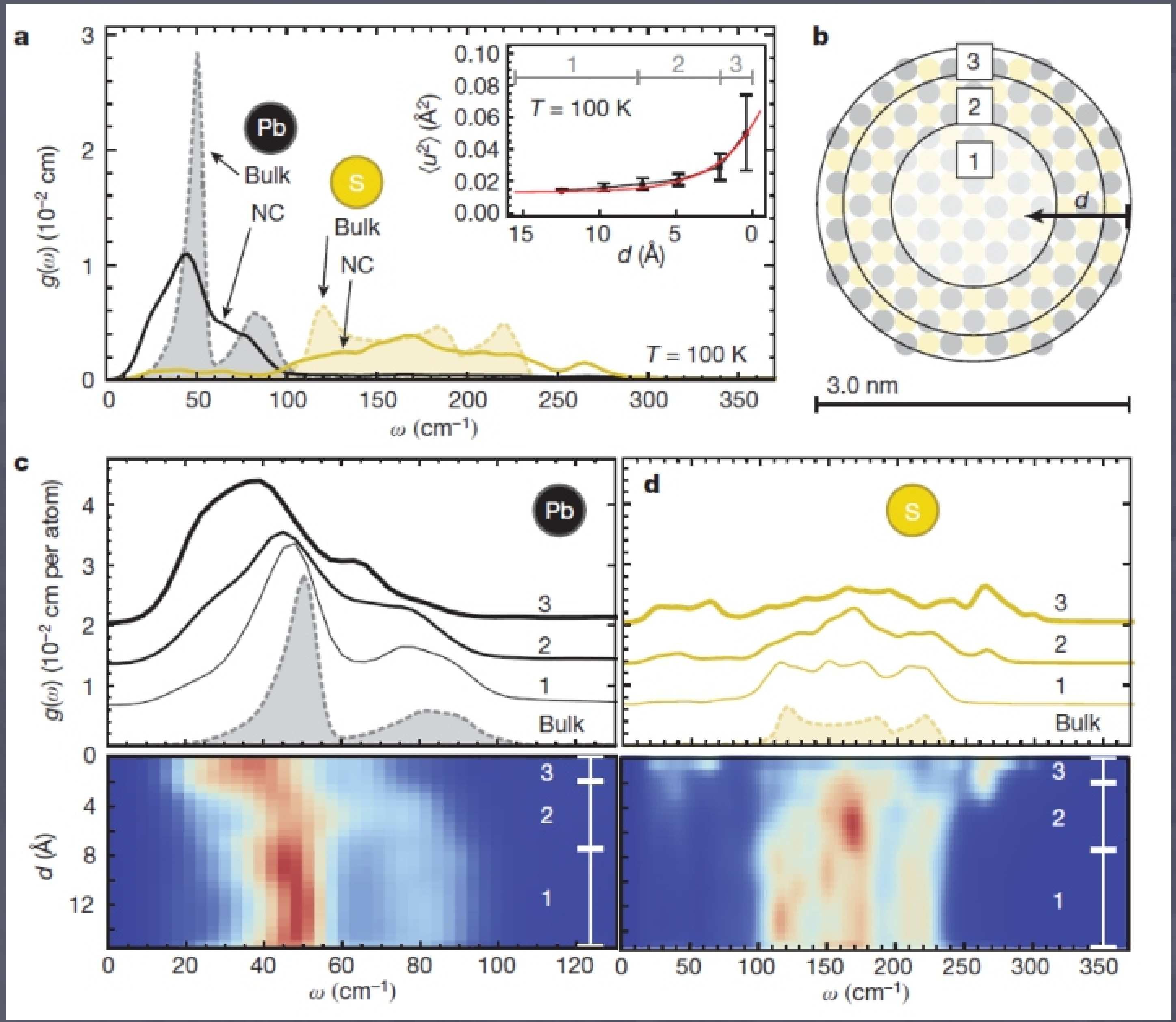
- Lead sulfide (PbS) nanoparticles are crucial from both fundamental scientific studies and technological applications.



- PbS nanoparticle-based photovoltaics (solar cells) have received a lot of attention an seen rapid advances in recent years.
- Relates to the fact that the band-gap of the material can be tuned by changing the size of the nano-particles.
- Improved understanding of these materials are however needed in order to optimize their performance in the functional device.

Surface Phonon Modes by INS

- By using inelastic neutron scattering (INS) the group of Prof. Vanessa Wood at ETHZ could show that below a certain nano-particle size, new phonon modes appear.

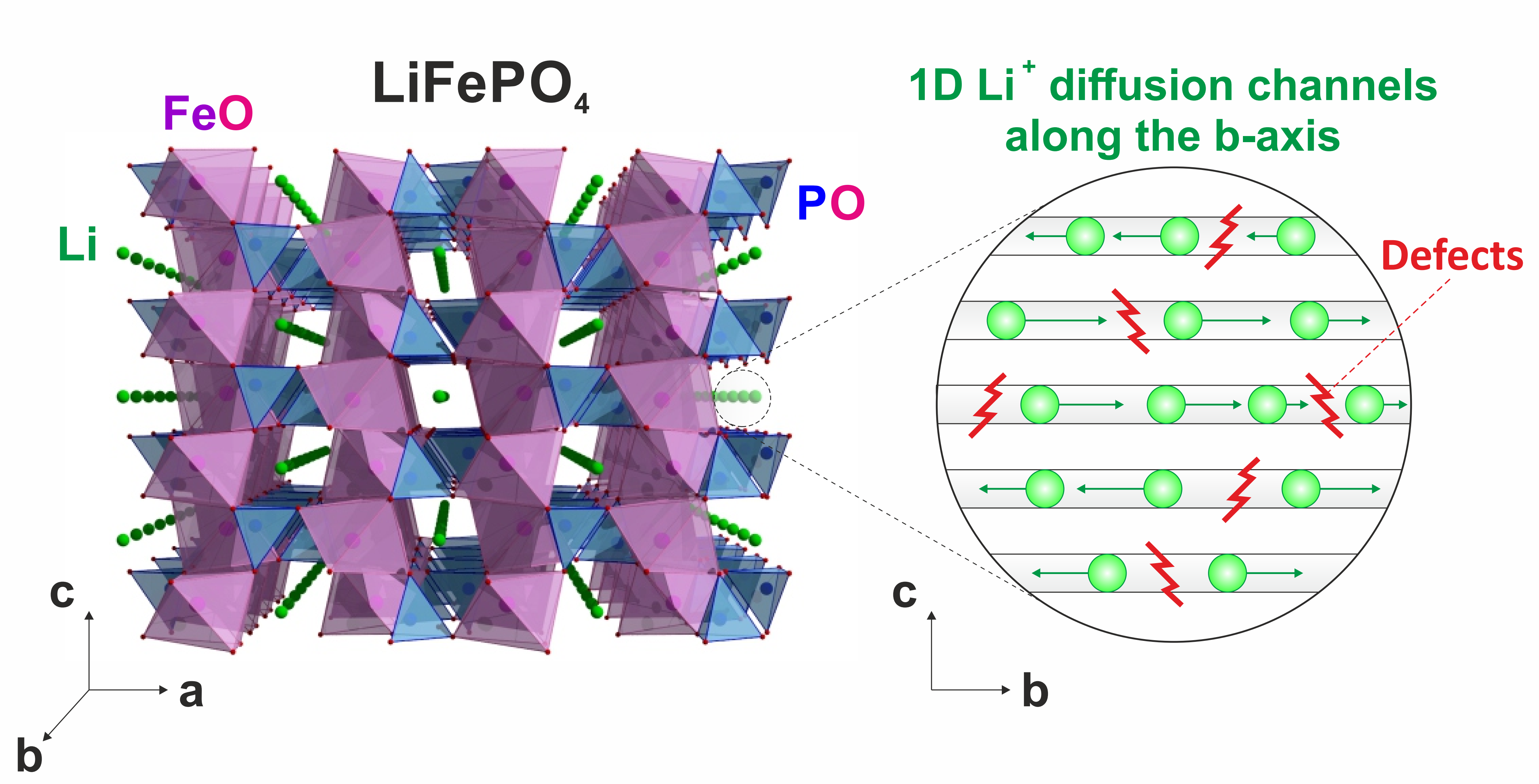


Nature 531, 618 (2016)

- *ab initio* molecular dynamics simulations were used to model the experimental INS data.
- This revealed that the new phonon modes exhibit both reduced symmetry and low energy owing to mechanical softness at the surface of the particles.
- These properties become important when phonons couple to electrons in actual devices.
- This improved understanding of phonon processes now allow for tailored nanomaterials, especially their surface treatments, in order to control and optimize the final device performance. **All thanks to INS!**

$LiFePO_4$ (LFPO)

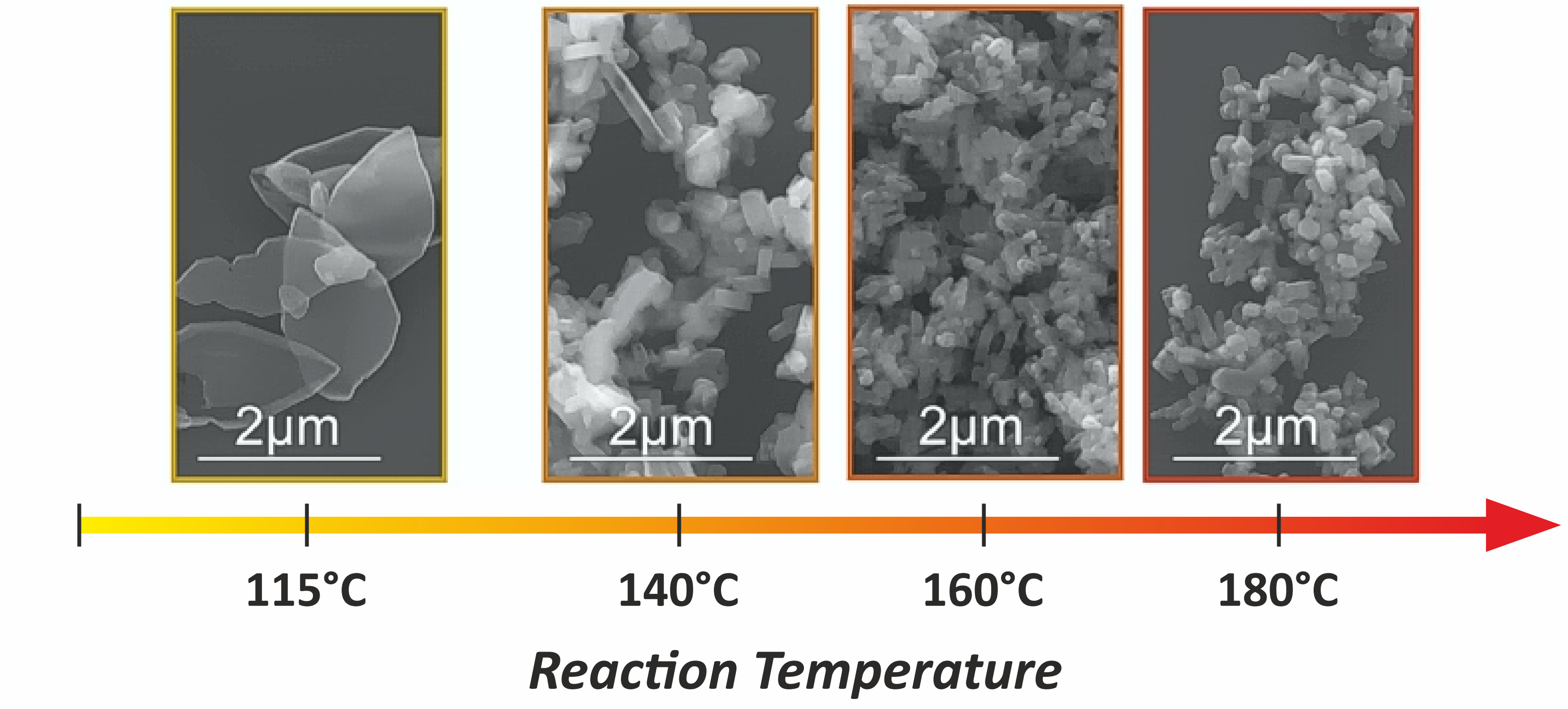
- The Phospho-olivine compound $LiFePO_4$ is currently a commercial battery cathode materials
- LFPO Display preferential Li-ion dynamics along the 1D diffusion channels parallel to the b-axis, which makes the Li-ion dynamics sensitive to defects in the diffusion channels.

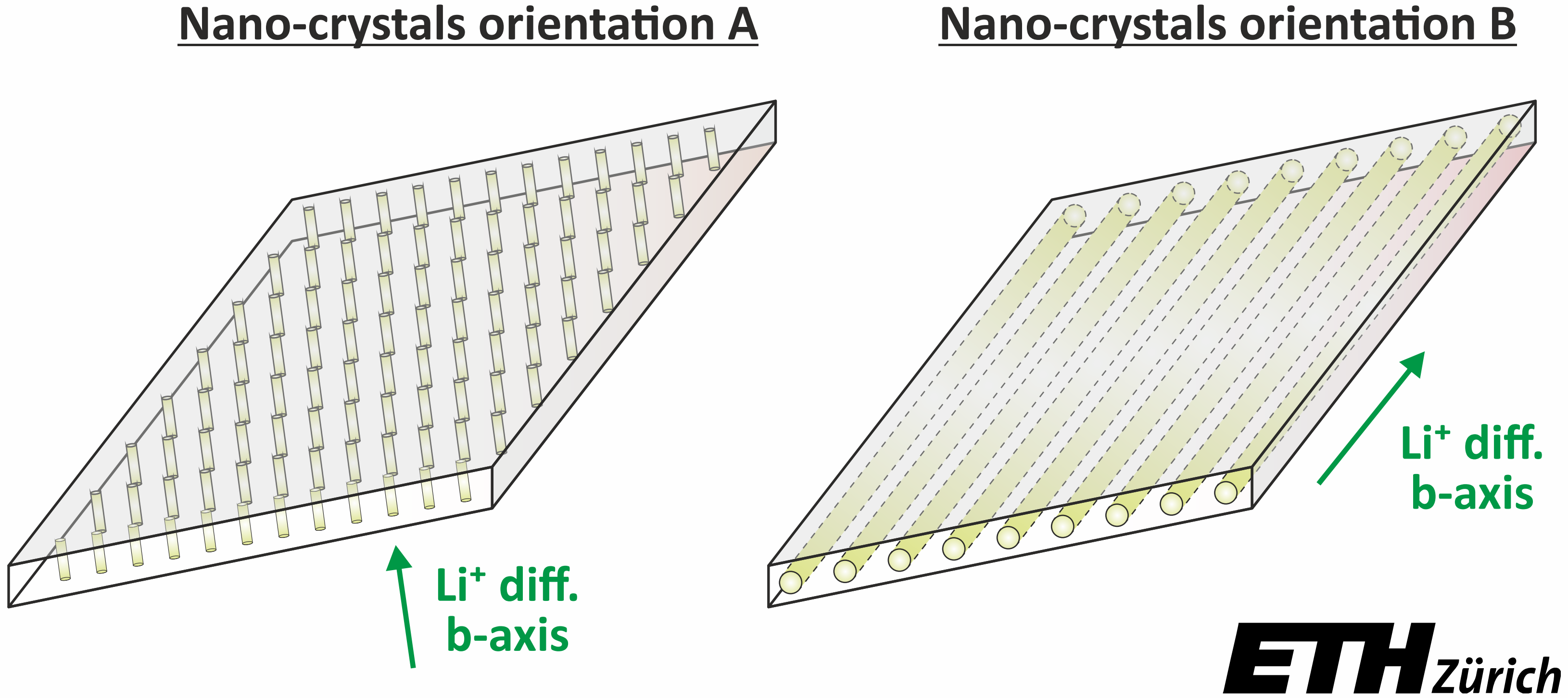


- We have already investigated this material in its bulk form and now...

Nano-structured LFPO

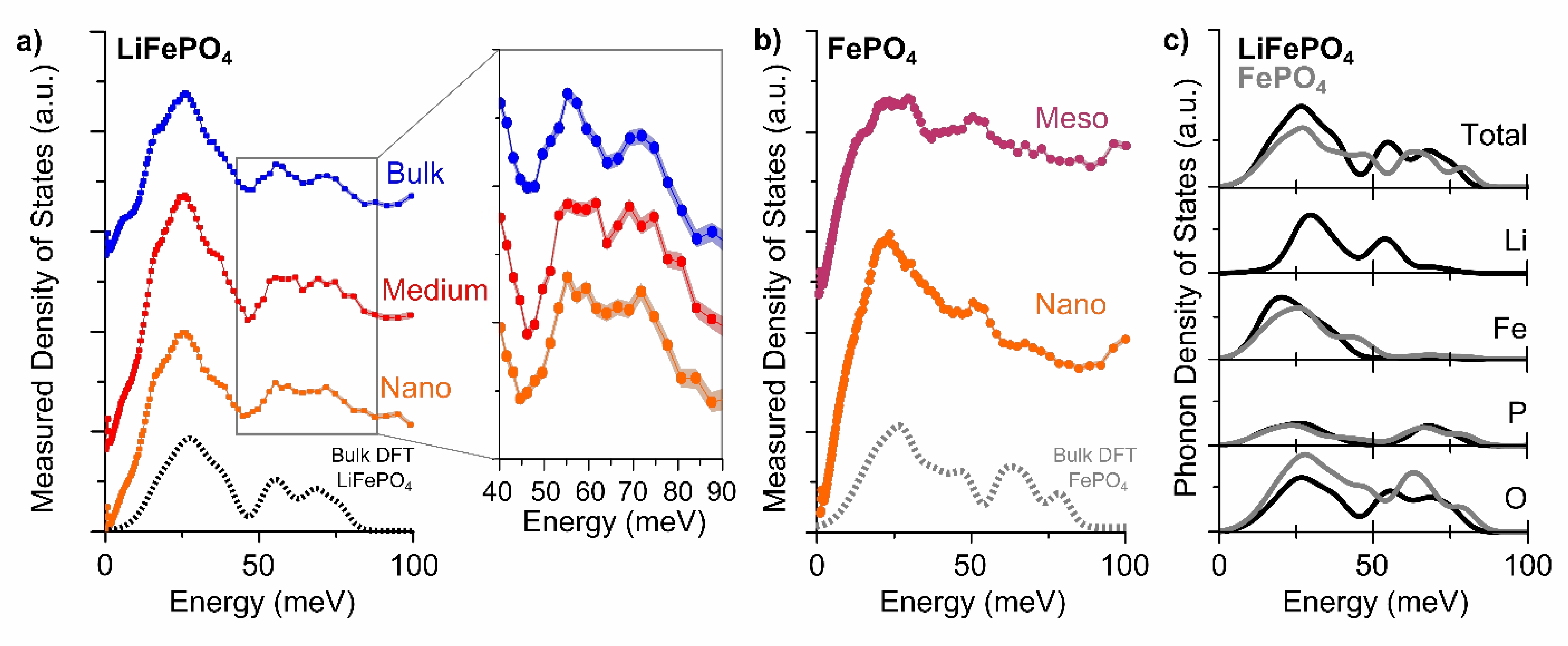
- Our collaborators at ETH Zürich (MaDE group of Prof. Vanessa Wood) are routinely producing LFPO nano-crystals.
- By varying the synthesis protocol they are able to tune not only the nano-platelet size but also the crystallographic (diffusion channel) direction.
- In a previous inelastic neutron scattering (INS) study [Nature 531, 618 (2016)] it was shown that nano-structured PbS display novel phonon modes below a certain crystal size. Such phonons are found to originate from the surface of the crystals (due to mechanical softening or strains)
- In our recent INS investigations we aimed to deduce if such phonons appears also in LFPO and if they affects the Li-ion diffusion.





INS of nano-LFPO

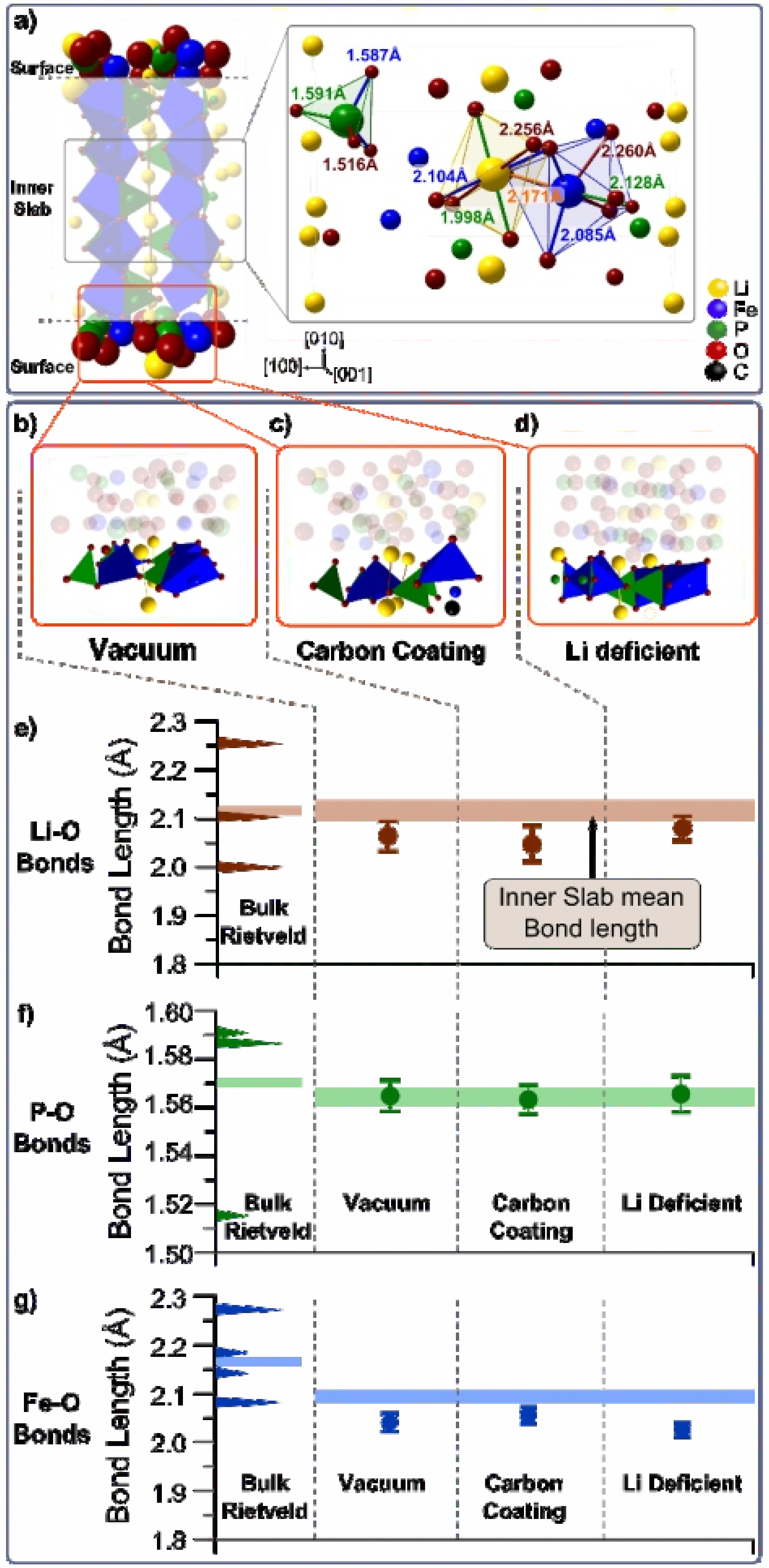
- Our very recent INS results show that the phonon spectrum changes when the size of the LFPO nano-platelets is reduced.



- Calculations of the elemental specific phonon density of states (PDOS) indicate that the changes in phonon modes (50-80 meV) are mainly related to the P-O as well as Li-O bonds.

DFT Calculations

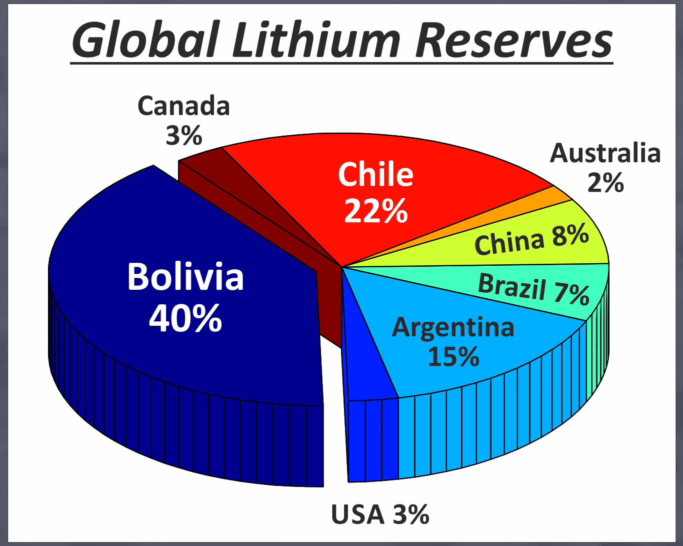
- More detailed *ab inition* simulations where performed for different surface termination of the LFPO nano-platelets.
- These calculations show that both the Li-O and Fe-O bonds are expected to shorten and are linked to surface reconstructions
- Of specific interest is the large reduction of the Li-O bond length for Carbon coated LFPO nano-crystals.
- Such reduction in Li-O bond length correlates well with the blue-shift of the phonon spectrum corresponding to the Li-O bond.
- Our results highlight how coatings can be used to systematically engineer the vibrations of atoms at the surface of battery active materials, and thereby impact lithium ion transport, charge transfer, and surface reactivity.

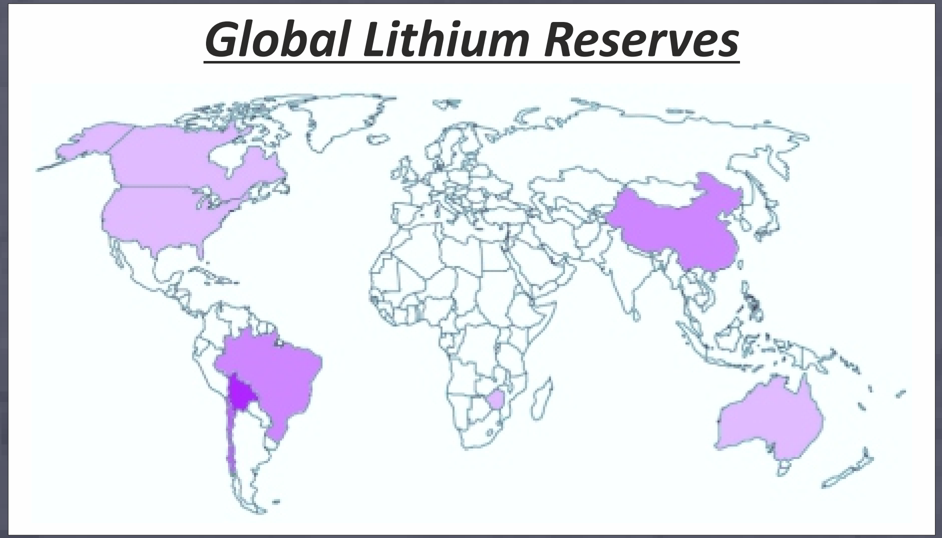


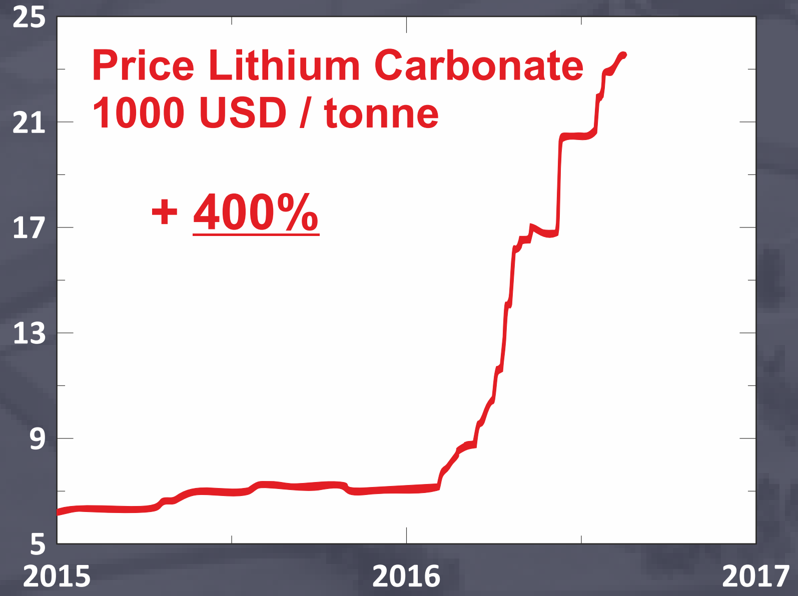
Benedek, Mansson, Wood, *et al.*, Sustainable Energy Fuels [RSC] 3, 508 (2019)

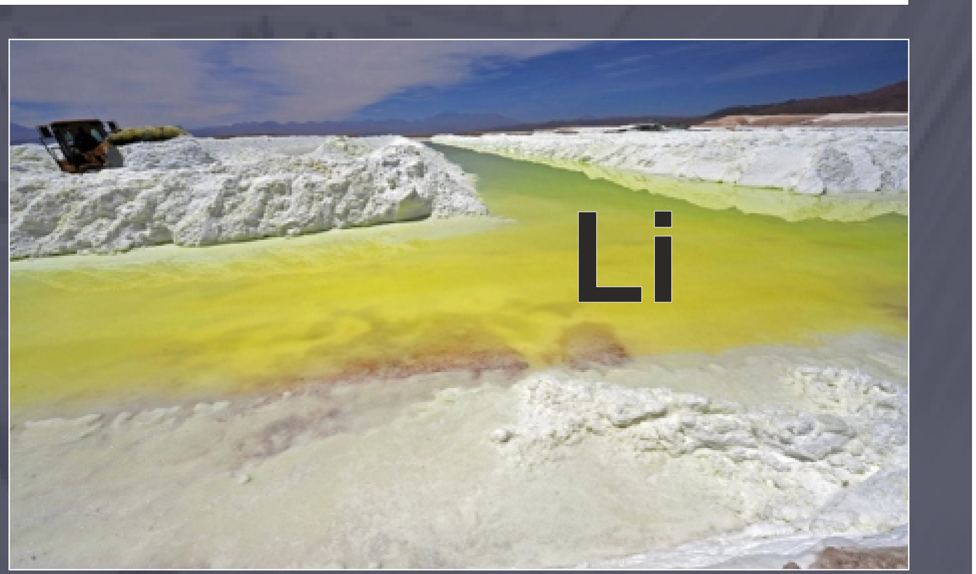
Lithium Ion Batteries

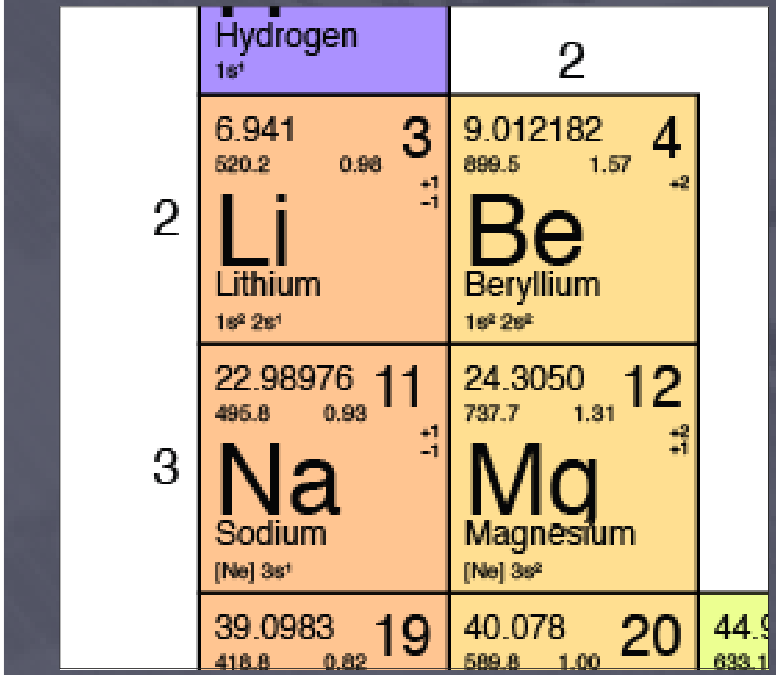
- Even before a general breakthrough of electrical cars, ~30% of Li-comsumption is for batteries.
- There are general concerns regarding the global Li-reserves and their 'geographical distribution'
- The process to extract Li is a nasty task that is not healthy for workers as well as environment
- Lithium alloys with many metals ® can only use expensive Cu (or Au) contacts in Li-ion batteries.











- Li-prize has tripled the last 5 years (2011: $4000 / ton → 2016: $14'000 / ton)

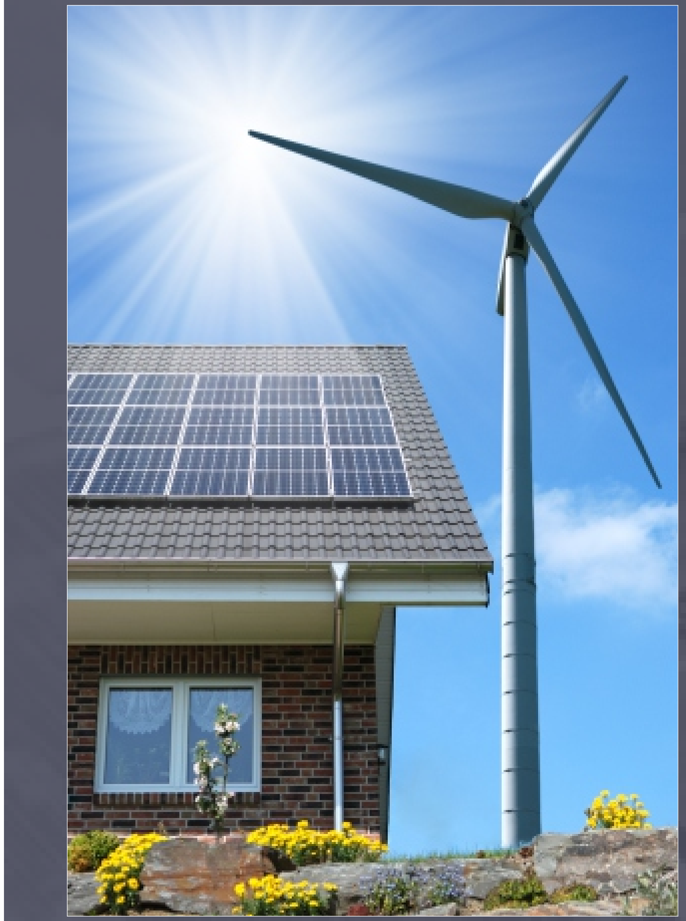
Will Lithium be the new oil ?!?!

- Should try to find some alternatives (not replacement).
- Take a step down the periodic table to Na...

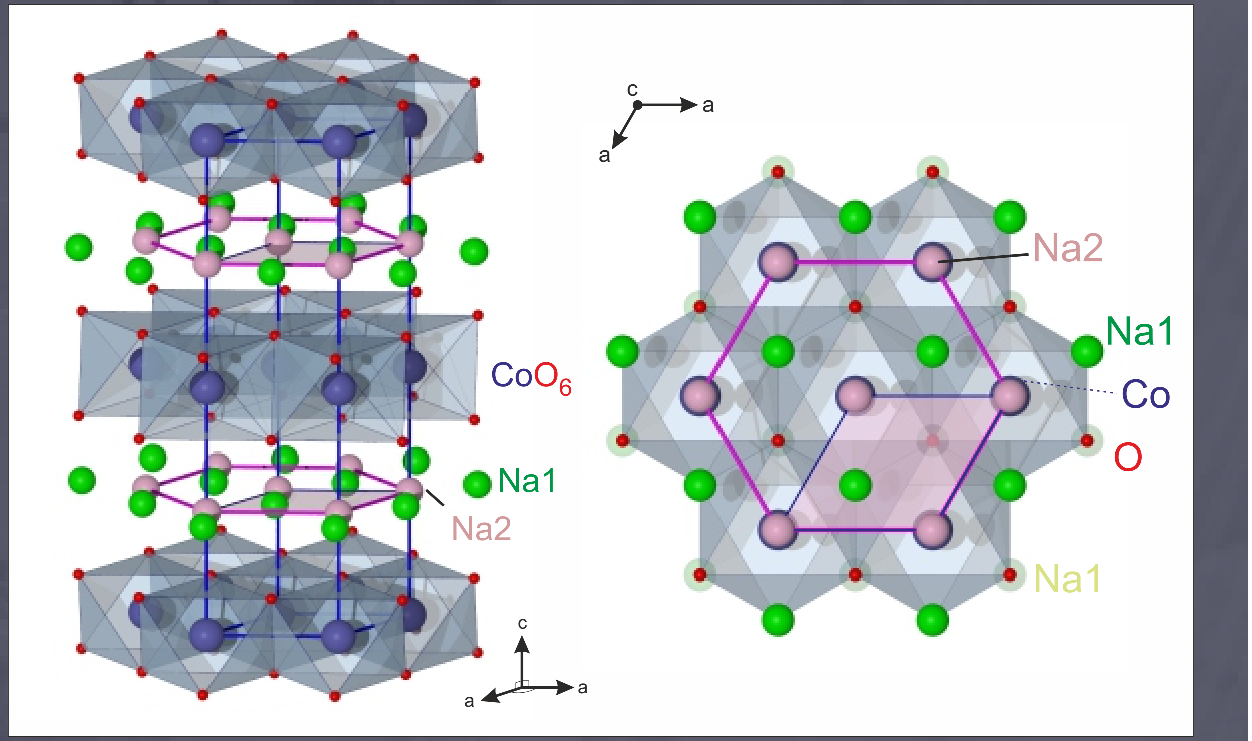
Sodium Ion Batteries

- Na is one of the most abundant elements in earth's crust (Na ≈ 23'600 ppm vs. Li ≈ 17 ppm) + the world ocean: *EIA is excellent for Na !*

- Sodium is the cheapest of all metals $500 / ton (= 30 × cheaper than Li).



- Na-batt's can use cheap Aluminium contacts.
- Na-batt's: 10 times cheaper, less toxic & easier to recycle *(initial development!)*.
- Na ions are larger (+70%) + lower operational voltage → Lower energy density and slower dynamics.
- Optimal for small-scale stationary storage of energy from solar panels, wind turbines and hydropower (*decentralized energy production & smart grids*)



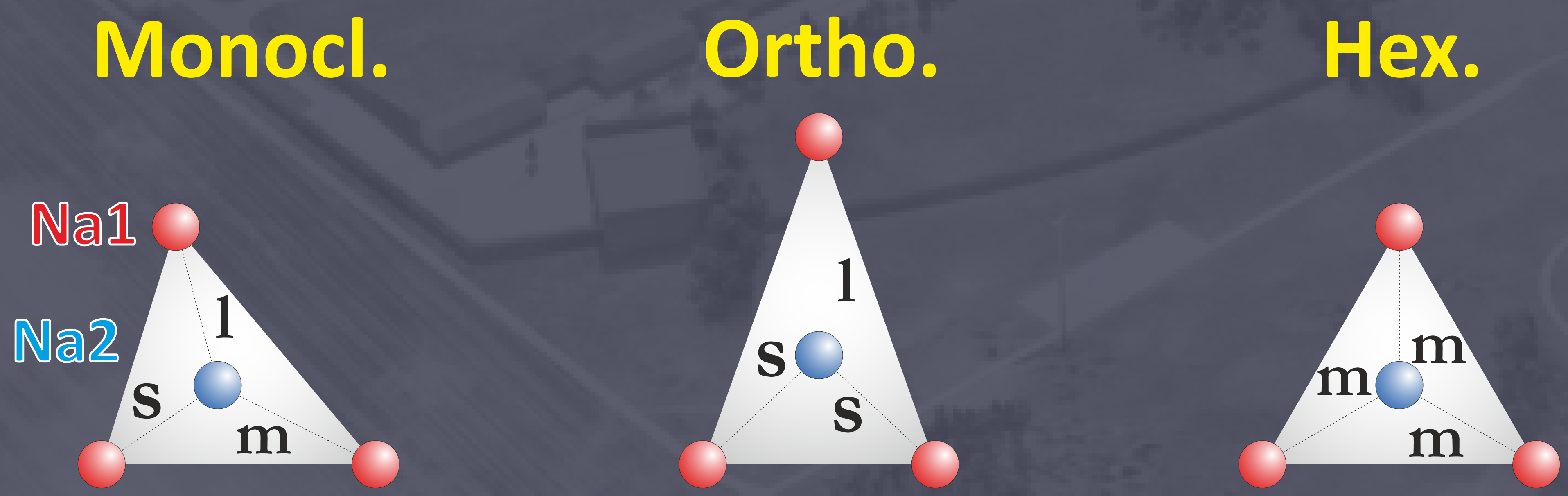
- Most common Li battery cathode material is $LiCoO_2$. To investigate the "Na-analog" i.e $NaCoO_2$ seems like a logical first step in order to understand Na-ion diffusion.

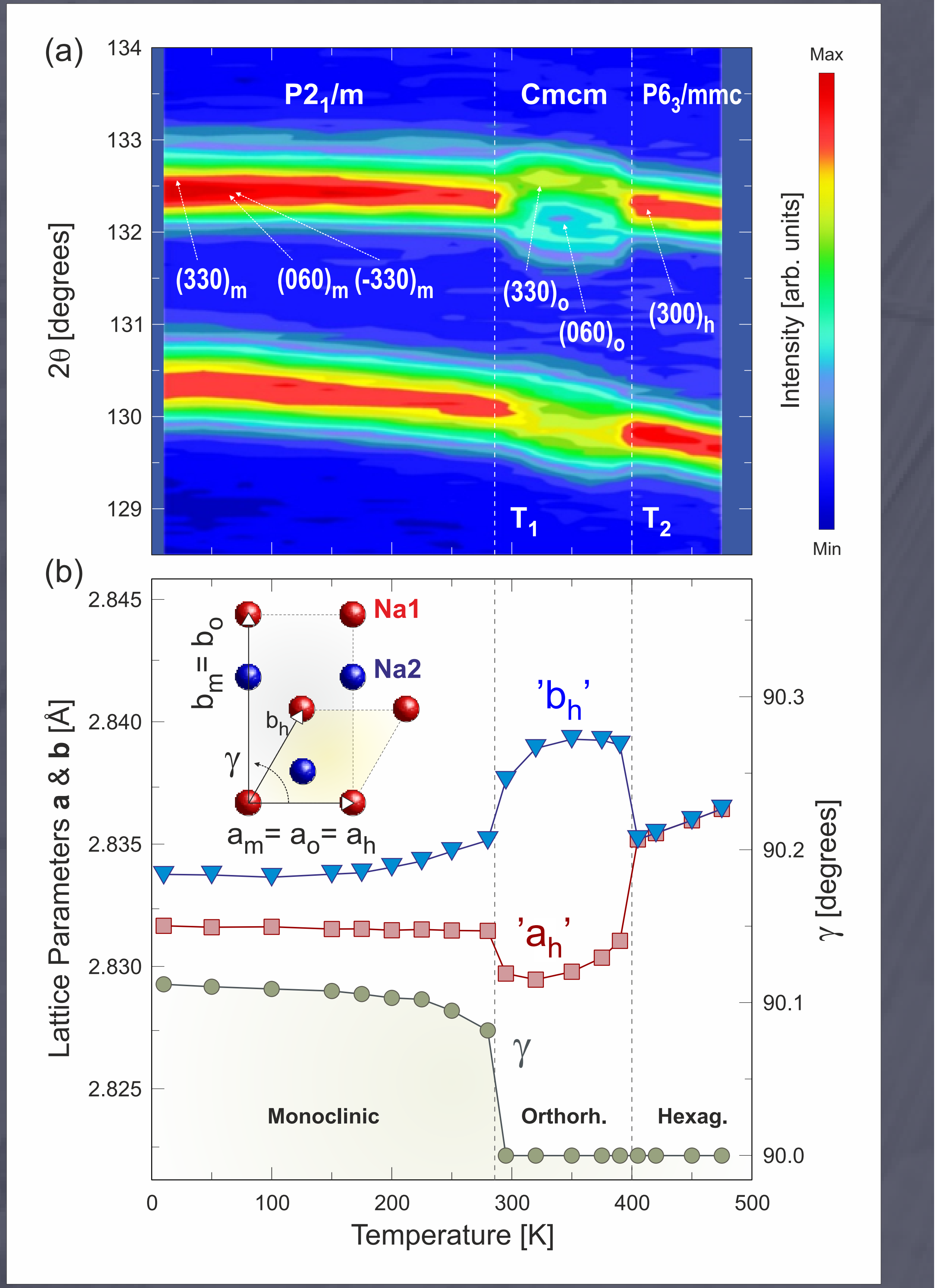
Neutron Powder Diffraction: $Na_{0.7}CoO_2$

- We have performed high-resolution neutron powder diffraction at the HRPT instrument, Paul Scherrer Institute (Switzerland)
- Neutrons (vs. x-rays) makes it easier to see the light Na-atoms.
- We find a series of subtle structural transitions as a function of *T*:

***T_1* = 290 K, Monoclinic to Orthorhombic**
***T_2* = 400 K, Orthorhombic to Hexagonal**

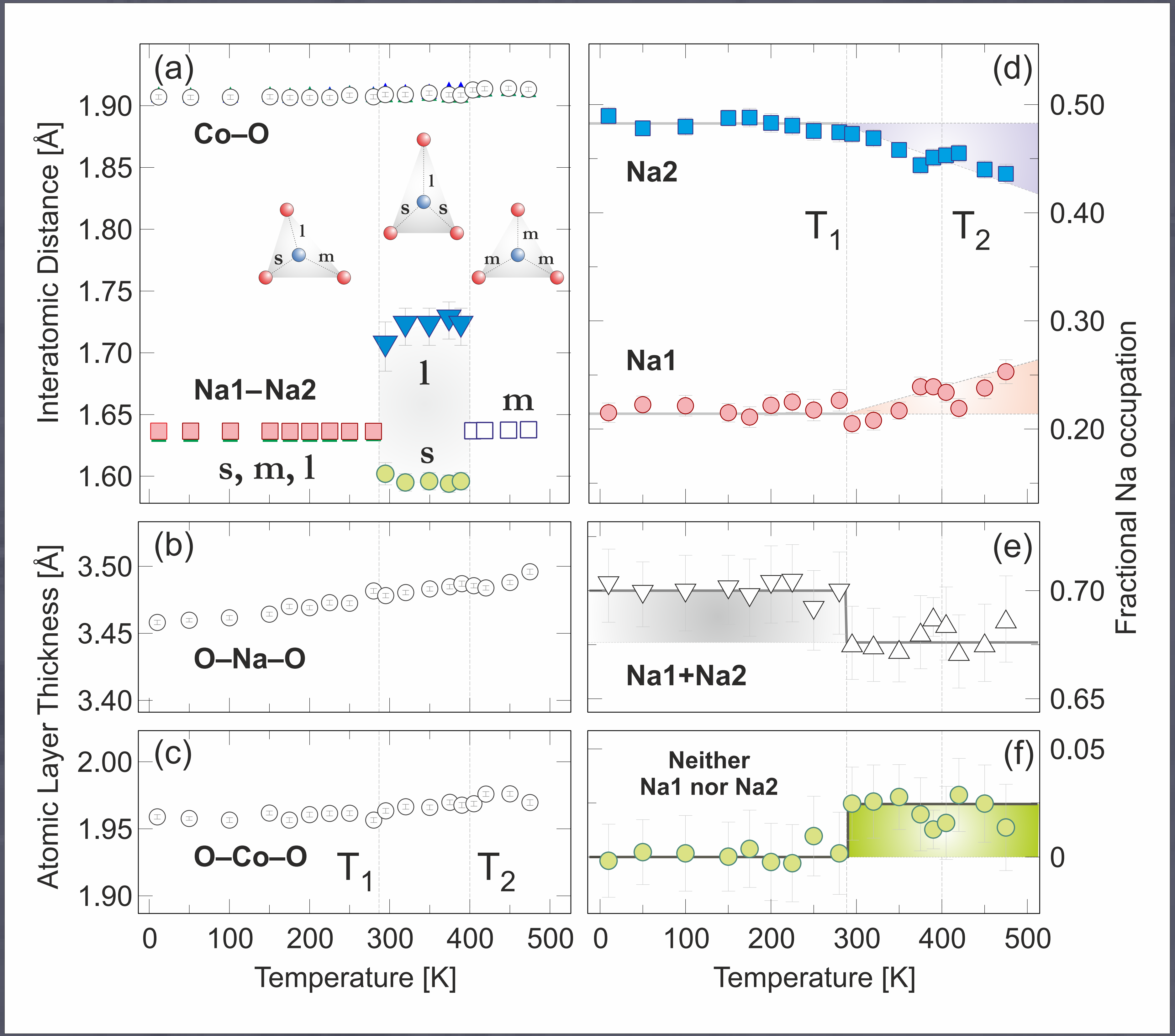
Here Na1-Na2 distances change:





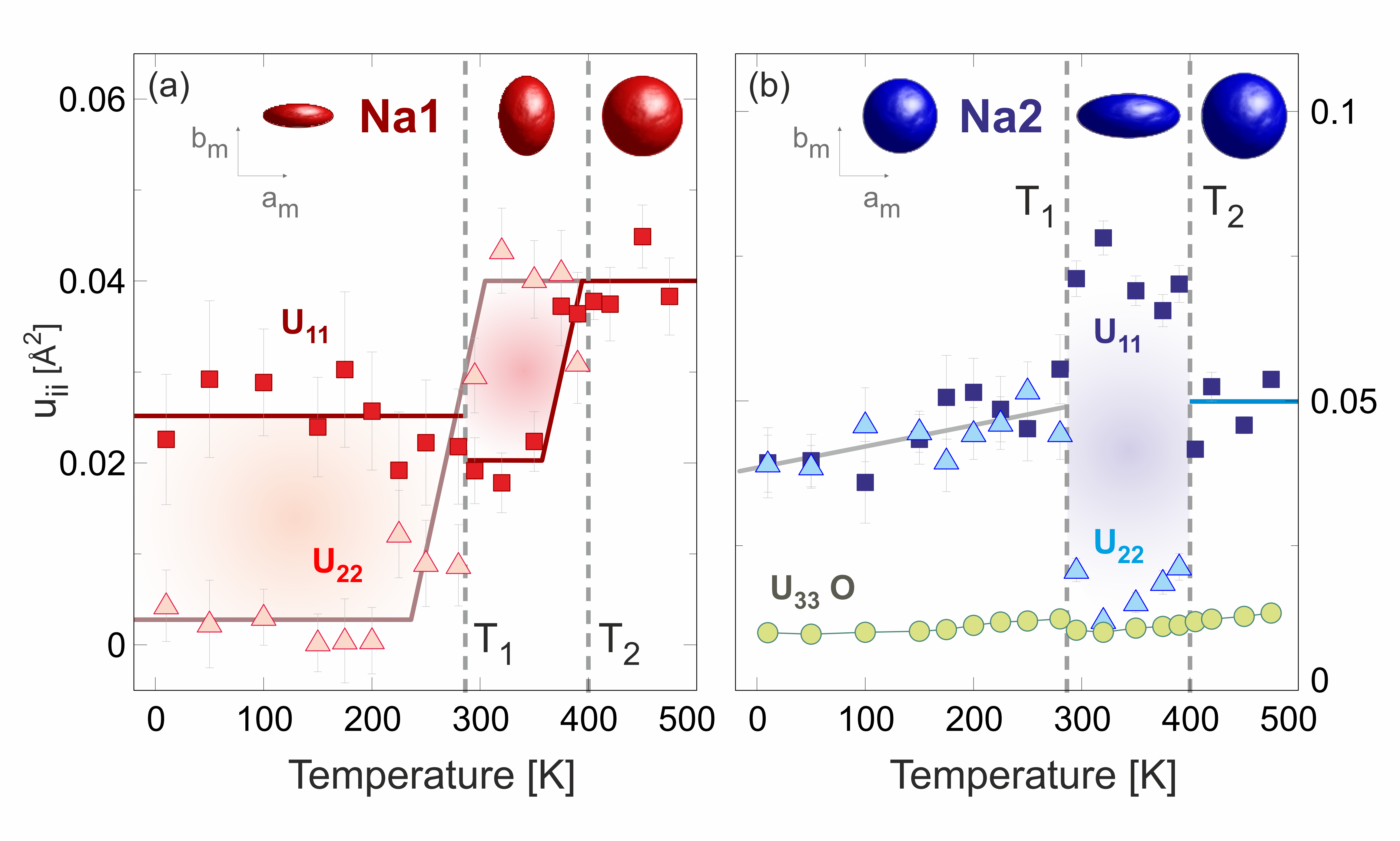
Fractional Na-site Occupancies

- Not only Na1-Na2 distances change but also the fractional Na-occupancies
- Na-ions are redistributed from Na2 to Na1 sites starting at ~T_1
- Total Na1+Na2 occupancy decrease i.e. Na-ions are somewhere else?!
- First indication that Na-ions are dynamic!



Debye-Waller Factors

- Temperature dependent DW factors reflect a reduction of Bragg intensities due to displacements of atoms from their equilibrium positions.

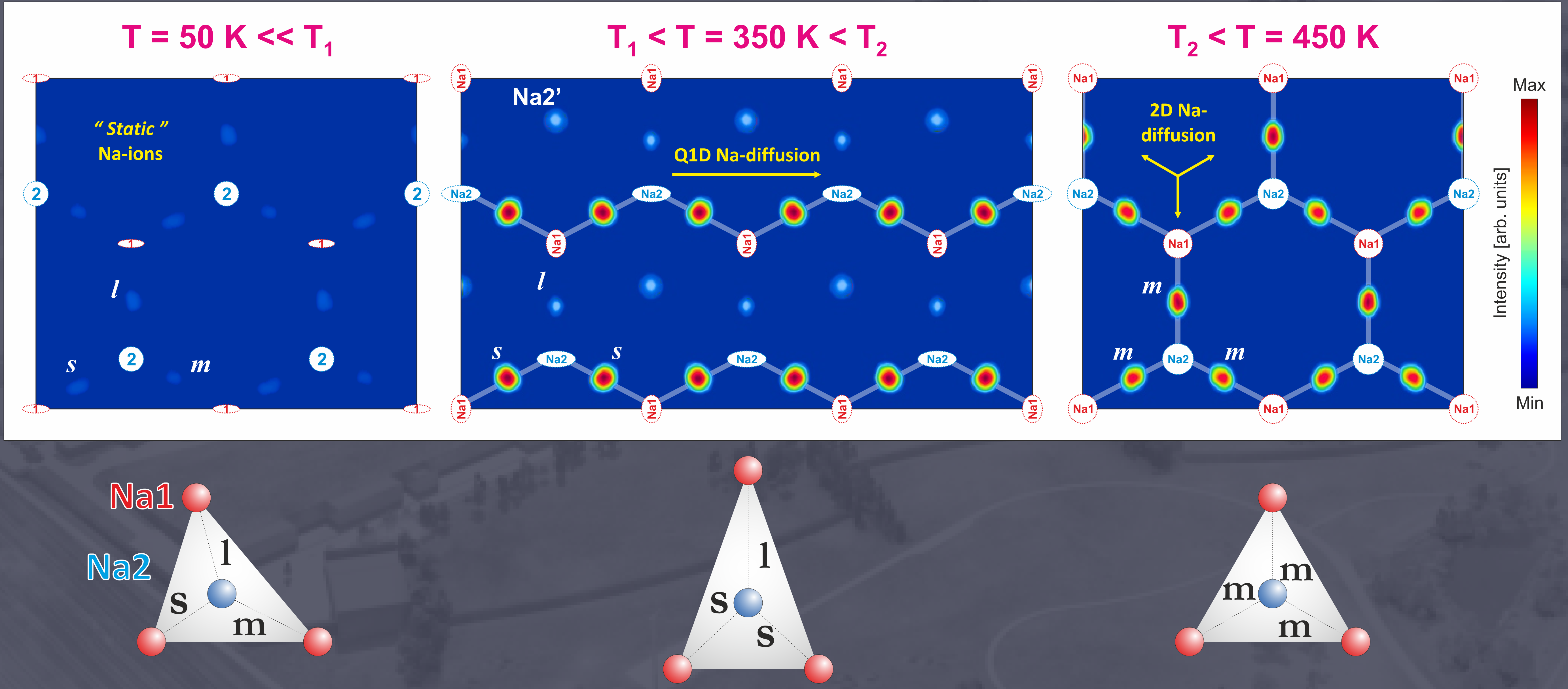


- The time averaged in-plane mean-square displacemets (u_{ii}) for Na-ions show clear anomalies around both T_1 and T_2.

- Anomaly is found also for the oxygen atoms, but it is clearly an order of magnitude smaller than for the Na-ions.

Fourier Analysis

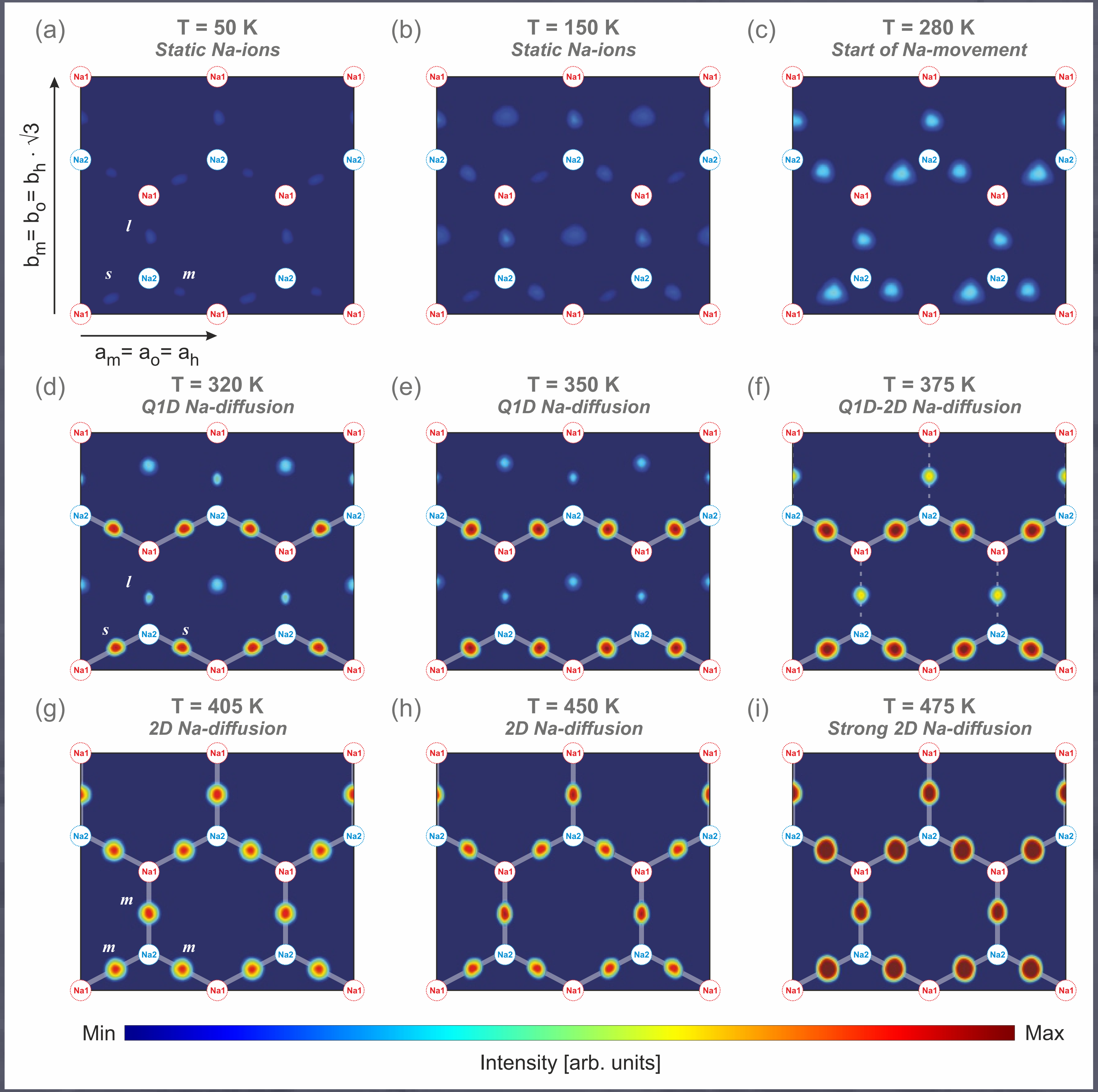
- Fourier difference maps provide information on residual scattering (in real space) contributing to the Bragg reflections not reproduced by the structural model.
- Na-layer maps show intriguing *T*-evolution: *'Static'* → *1D Na-diffusion* → *2D Na-diffusion*



***Physical Review Letters* 110, 266401 (2013)**

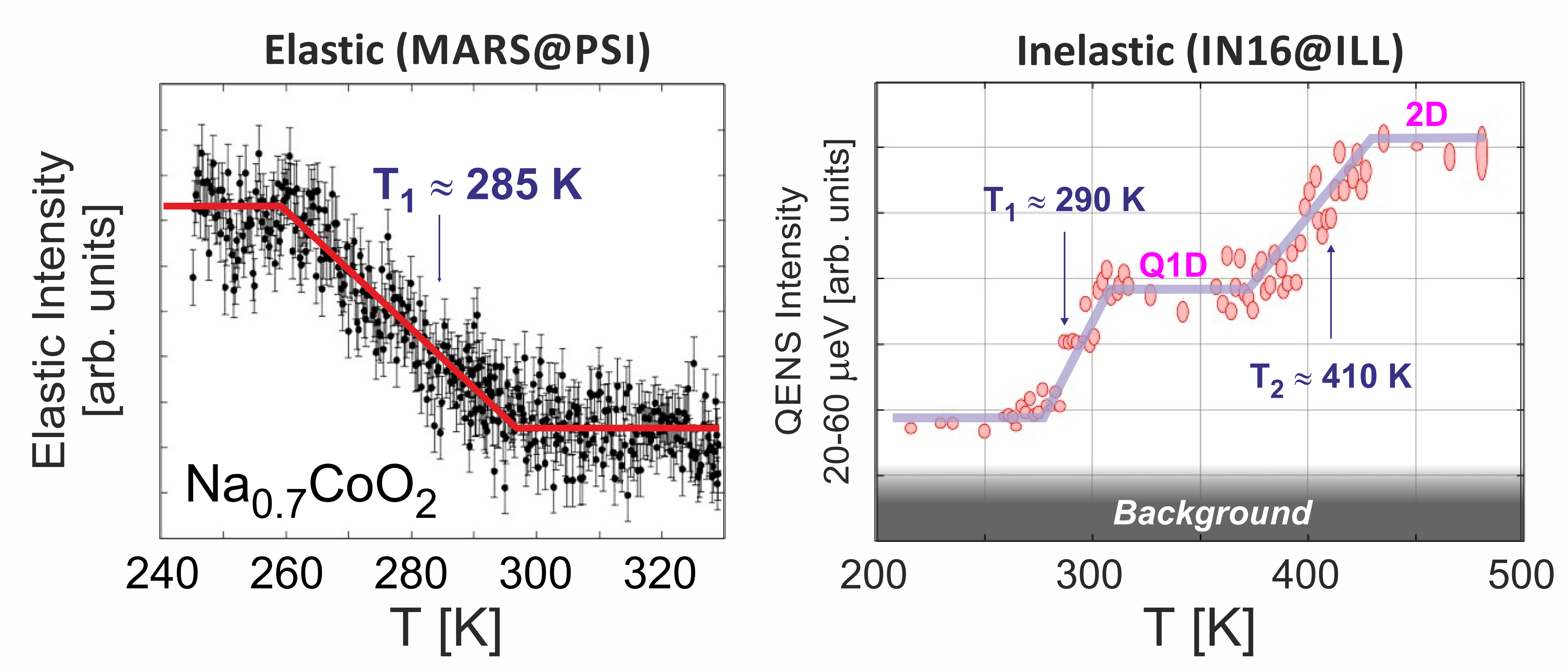
- Evolution of diffusion mechanism is strongly linked to Na1-Na2 distances through the subtle structural transitions (that open the diffusion channels).

Complete Temperature Dependence



Quasi-Elastic Neutron Scattering (QENS)

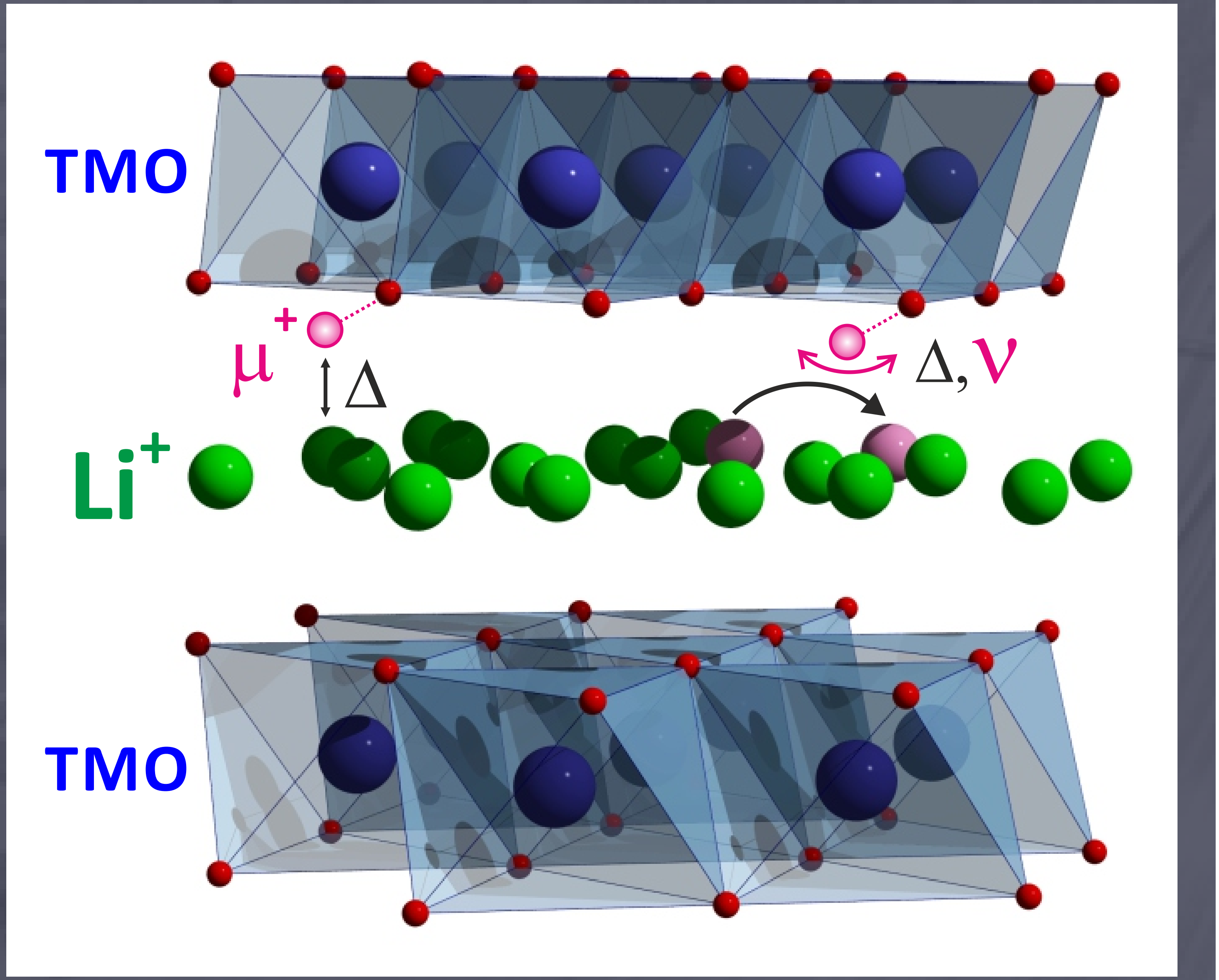
- Energy-resolved neutron scattering giving direct access to ion-dynamics (isotope sensitive!)
- We have performed a preliminary QENS study of $Na_{0.7}CoO_2$, which show a decrease in elastic intensity around T_1 = 285 K as well as a simultanous increase in QENS intensity
- A second step is visible around T_2 = 400 K (1D-to-2D diffusion!), fully constistent with NPD, **We are currently conducting Q-dependent QENS studis** (details on the diffusion mechanism)

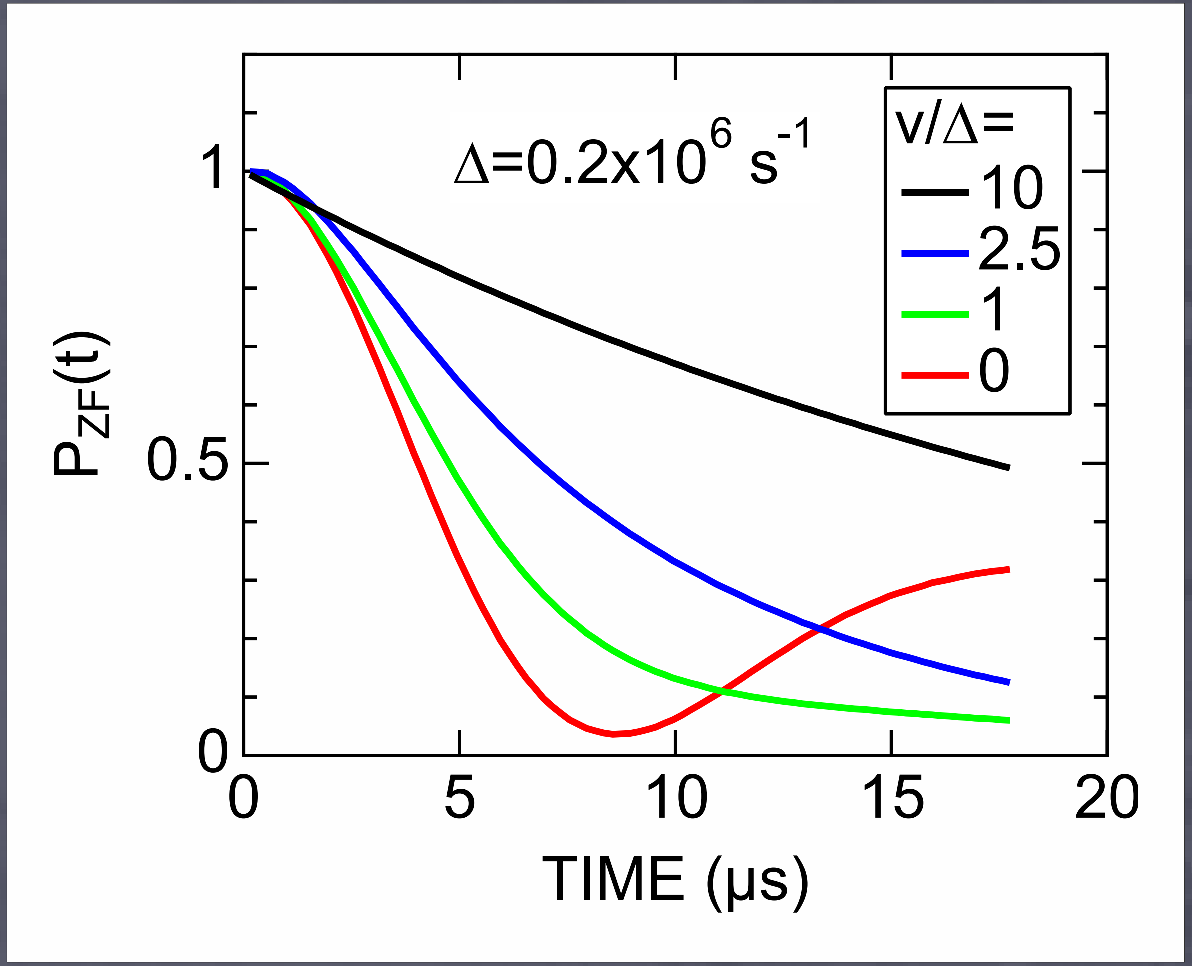


EPJ Web of Conf. 83, 02008 (2015)

Ion Diffusion by μ^+SR

- Muons are very sensitive probes of local internal fields
- In the paramagnetic state, muons feel mainly the random nuclear dipole fields (of Li) → Δ
- Implanted μ^+ bind strongly to O^- within the crystal lattice
- If Li-ions are immobile the mSR time-spectrum is described by a static **Kubo-Toyabe** function

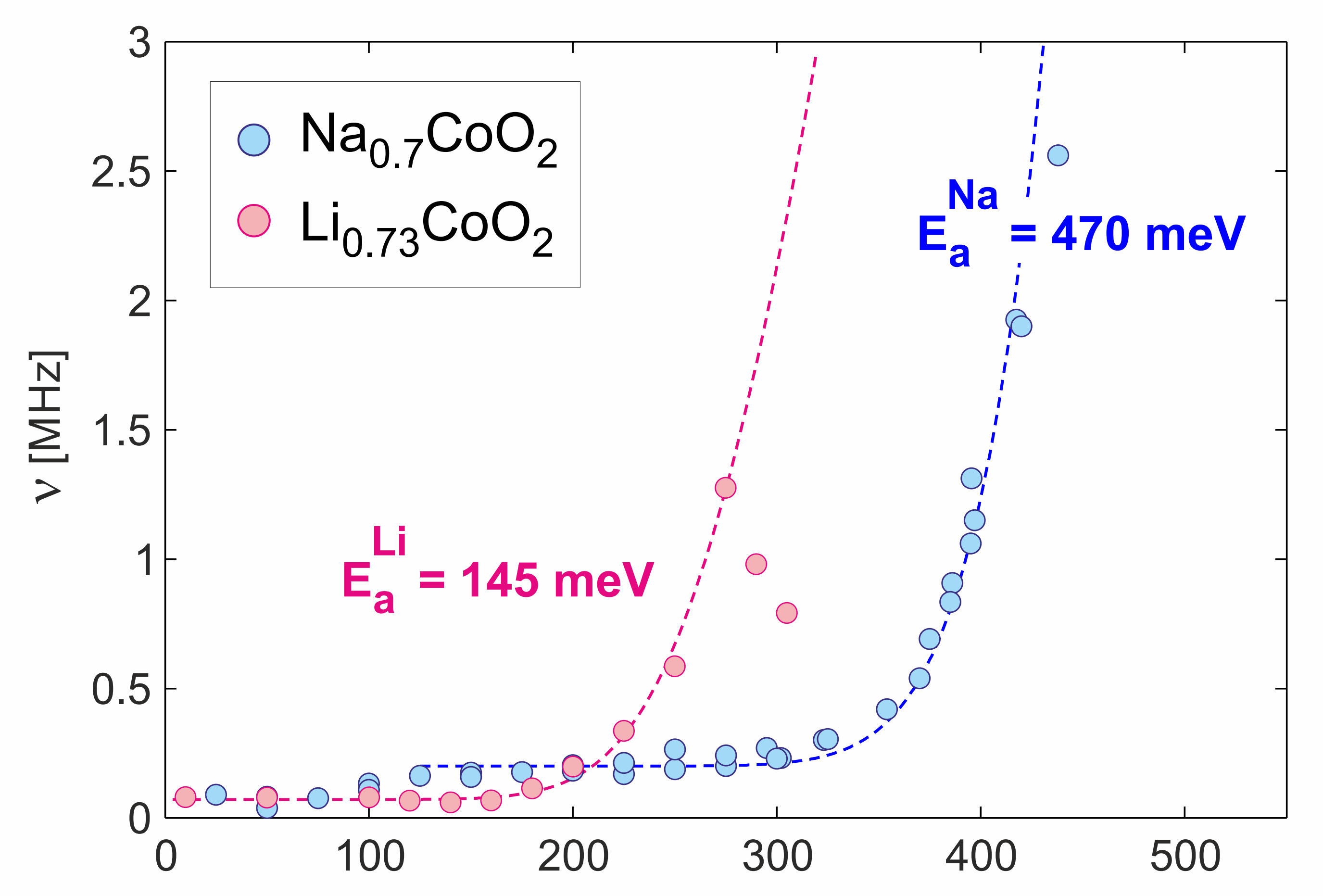


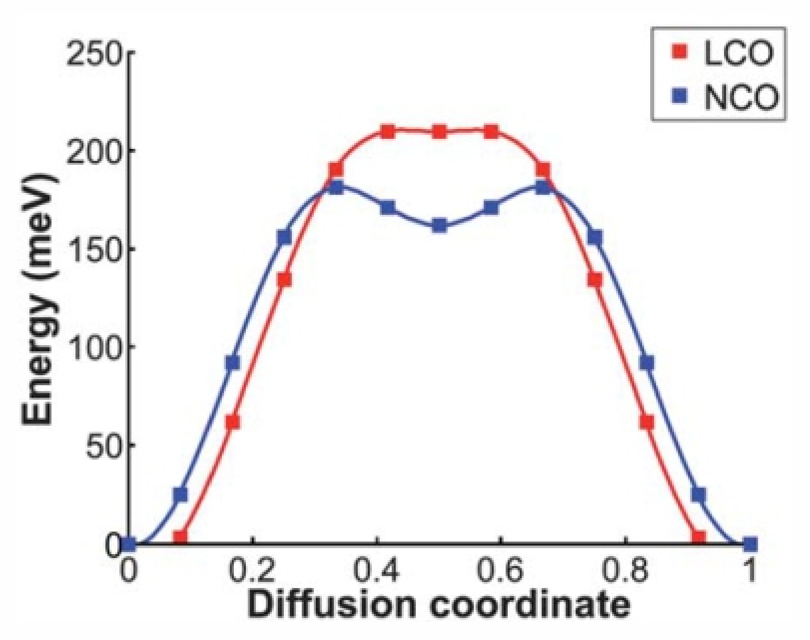


- If ion-diffusion is present, the muons will detect a dynamic contribution to the dipole field.
- Data is now described by a dynamic KT function that includes the parameter: **ion hopping rate (ν)**
- From *T*-dependence ν(*T*), the ion self-diffusion coefficient (**D_{ion}**) is extracted

Na-ion Diffusion by μ^+SR

- The hopping-rate (ν) show a clear diffusive behavior for $T \geq 300$ K and is well fitted to an Arrhenius equation.
- We can extract E_a(Na) = 470 meV.
- This is 3 time larger than our results from $Li_{0.7}CoO_2$.





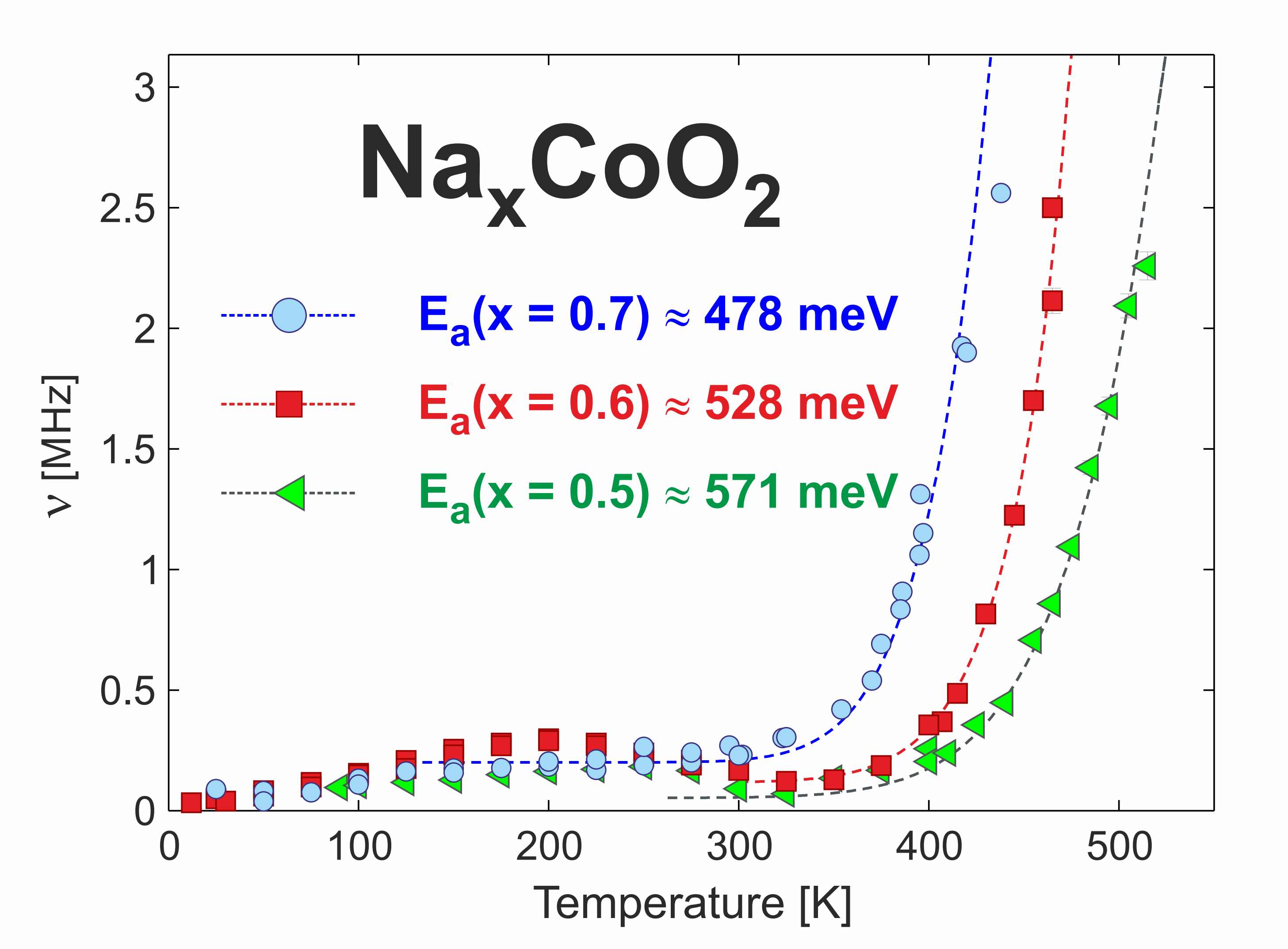
Ceder *et al.*
Energy Environ. Sci.
4, 3680 (2011)

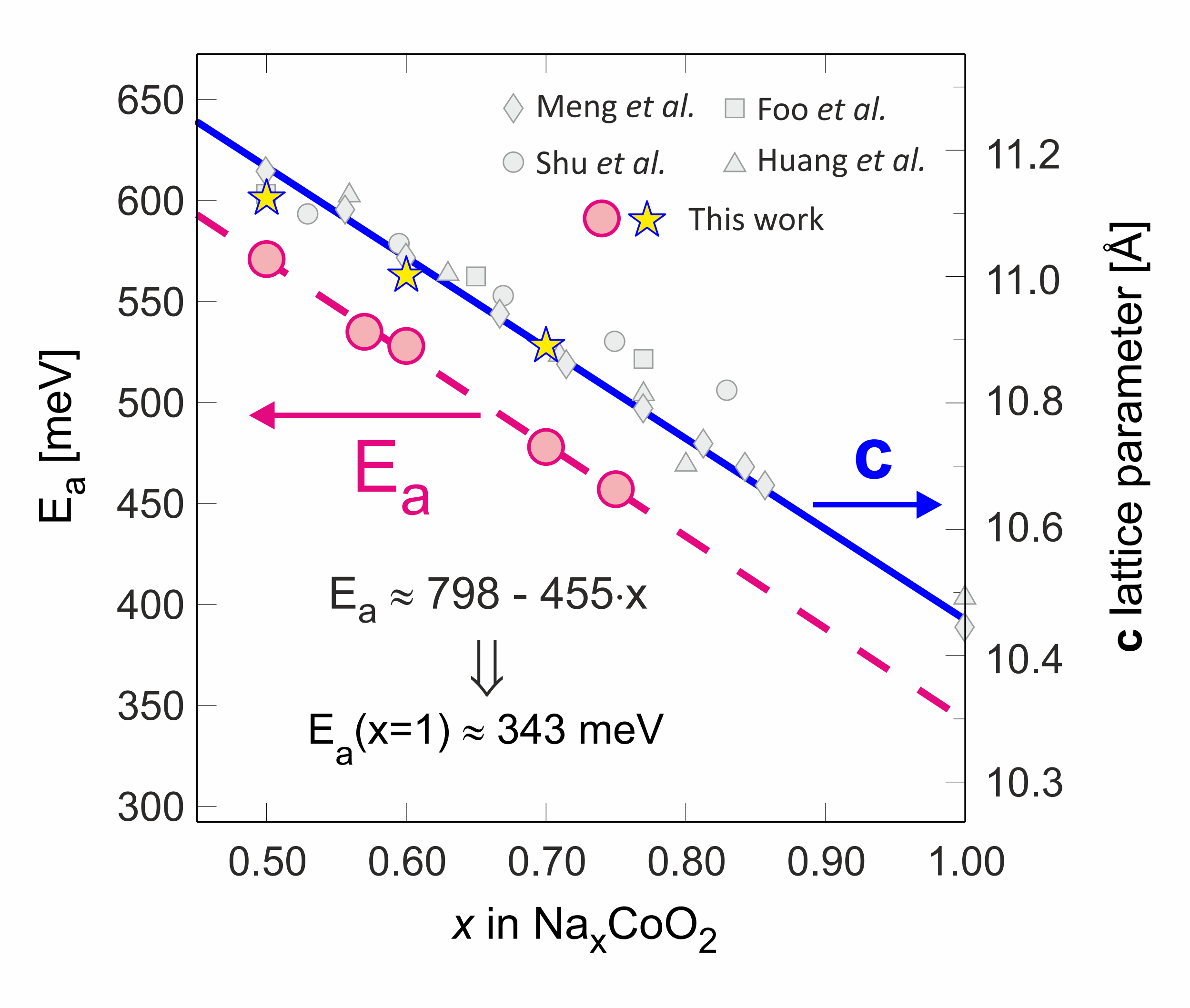
- Such results are rather surprising since *ab initio* calculations indicate that E_a for Li/$NaCoO_2$ should be similar or even lower for Na-ions.
- Explanation: error in model input *e.g.* the crystal structure (not simple hexagonal for $NaCoO_2$)
- Applying same procedure as for $LiCoO_2$ → Na-diffusion coefficient (D_{Na}) as a function of T:

$$D_{Na}(400\ \mathrm{K}) = 3.10\times10^{-10}\ \mathrm{cm}^2/\mathrm{s} \qquad D_{Na}(300\ \mathrm{K}) = 4.60\times10^{-11}\ \mathrm{cm}^2/\mathrm{s}$$

Na-/x-dependence

- We also performed measurements for samples with different Na-content (*x*)
- Strong dependence on the onset of Na-ion diffusion with *x*
- Activation energy (E_a) decreases with increasing sodium content and scales inverse linearly with *x*.

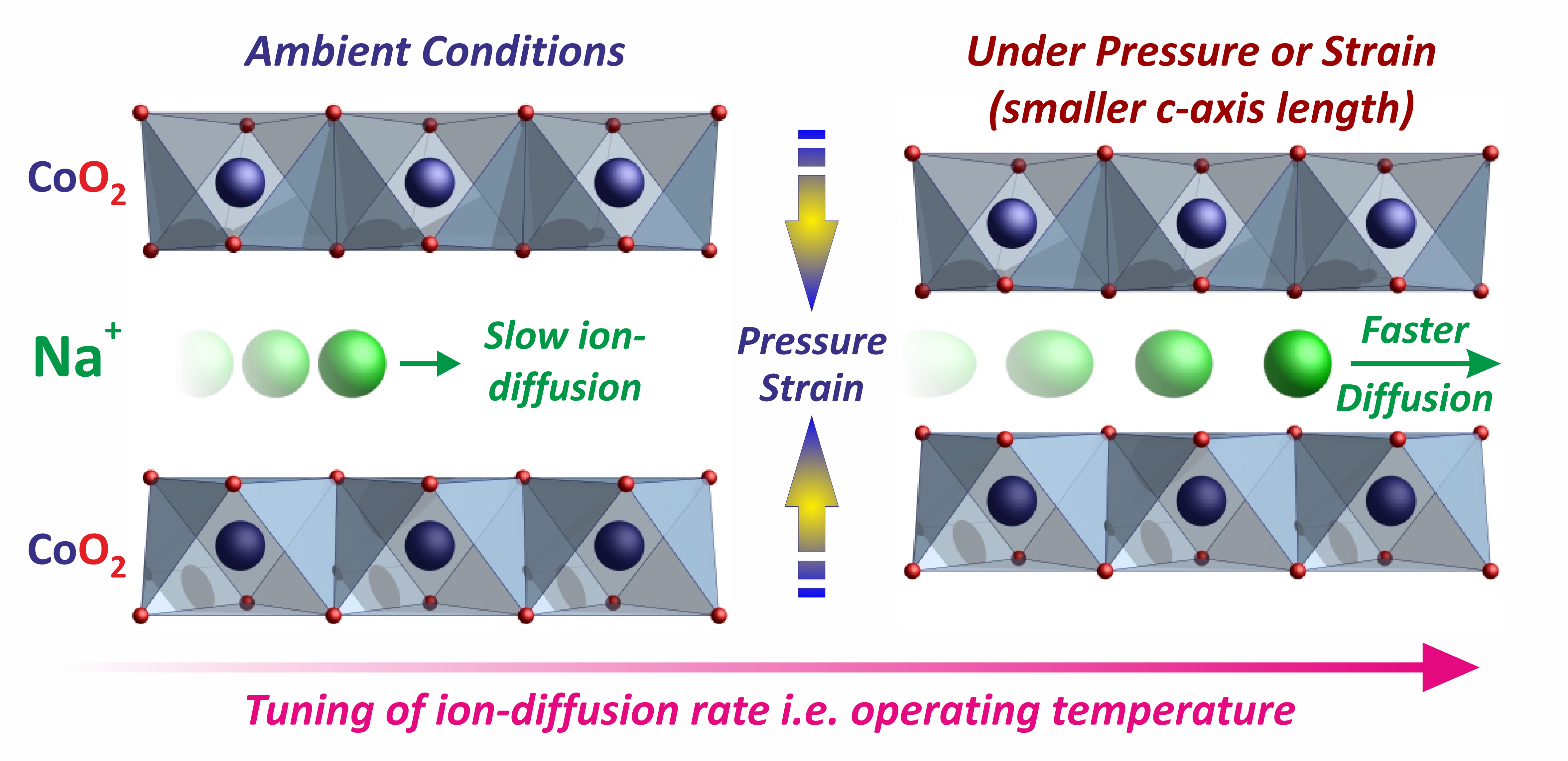




- For this compound it is well known that the length of c-axis scales in the same way as E_a with *x*.
- Counter-intuitive increase of Na-diffusion (D_{Na}) with shorter c-axis !?
- Can we use this knowledge to tune ion-diffusion in battery compounds?!

Pressure Tuning Possibility ?!

- P = 15 kbar is only a 0.5% lattice strain ⇒ ΔT = 20 K
- 2.5% strain is very feasible for thin films ⇒ ΔT = 100 K = *material usable at RT or NOT !!!*
- Exponential T-dependence for diffusion-rate = *device performance using same material !!!*

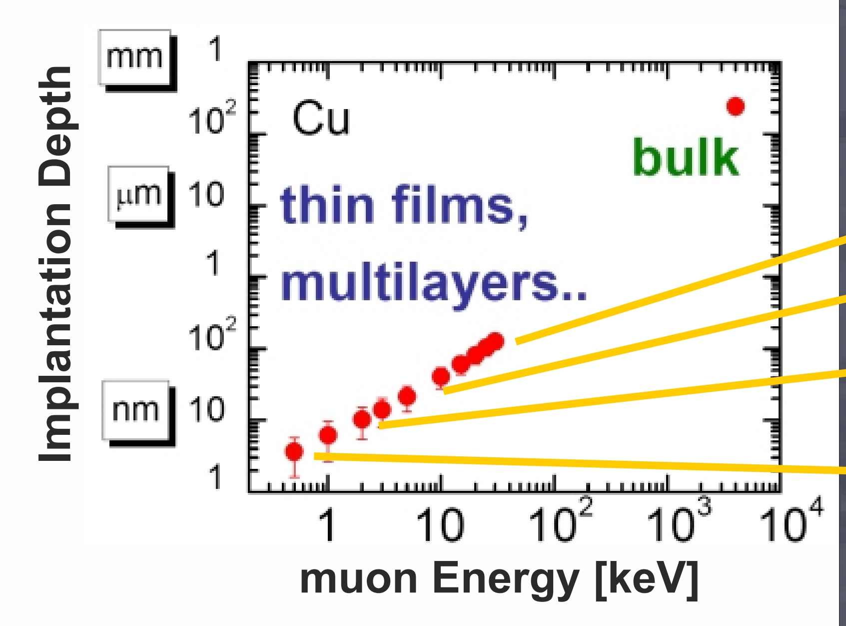


- Open a new dimension for thin film or nano-structured batteries using either new materials or 'old rejected ones' that can be of re-evaluated.

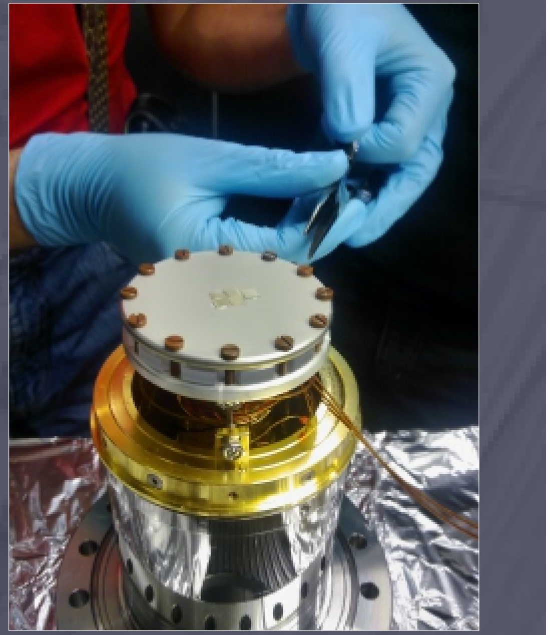
Low-Energy μ^+SR (LEM)

- The extension to our method is to use low-energy μ^+SR (LEM) to investigate future thin film batteries in a straightforward manner.

- By tuning the muon implantation depth one can study ion-diffusion in all the individual components of the device, <u>including their interfaces</u> !!!



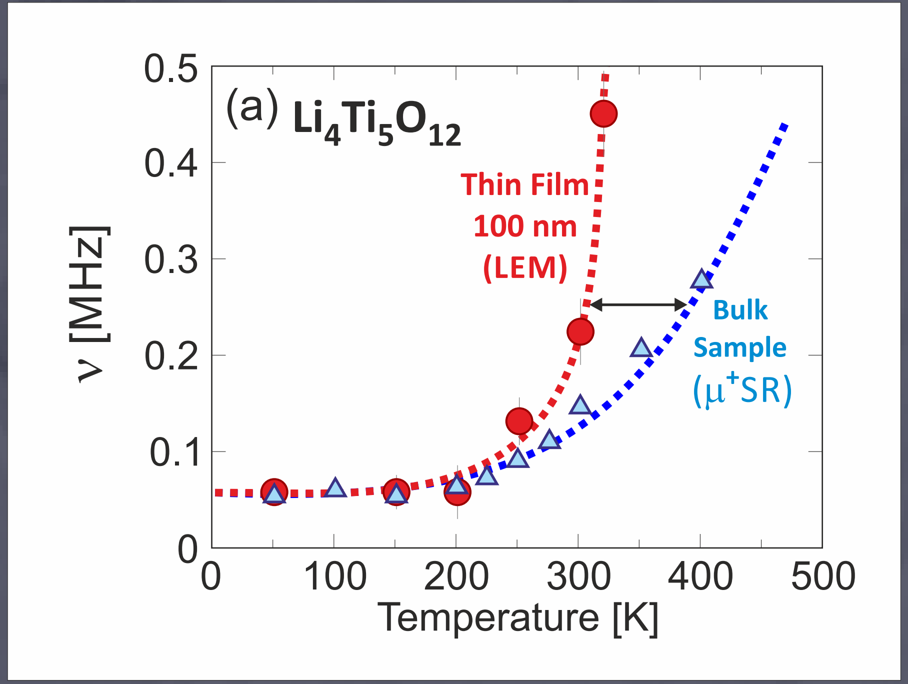
Thin film Battery



- This also allows for investigations on how low-dimensionality affects ion diffusion (i.e. thin film vs. bulk material).

- Our recent data from LEM@PSI in fact show a higher diffusion rate in a 100 nm thin $Li_4Ti_5O_{12}$ film than in bulk samples.

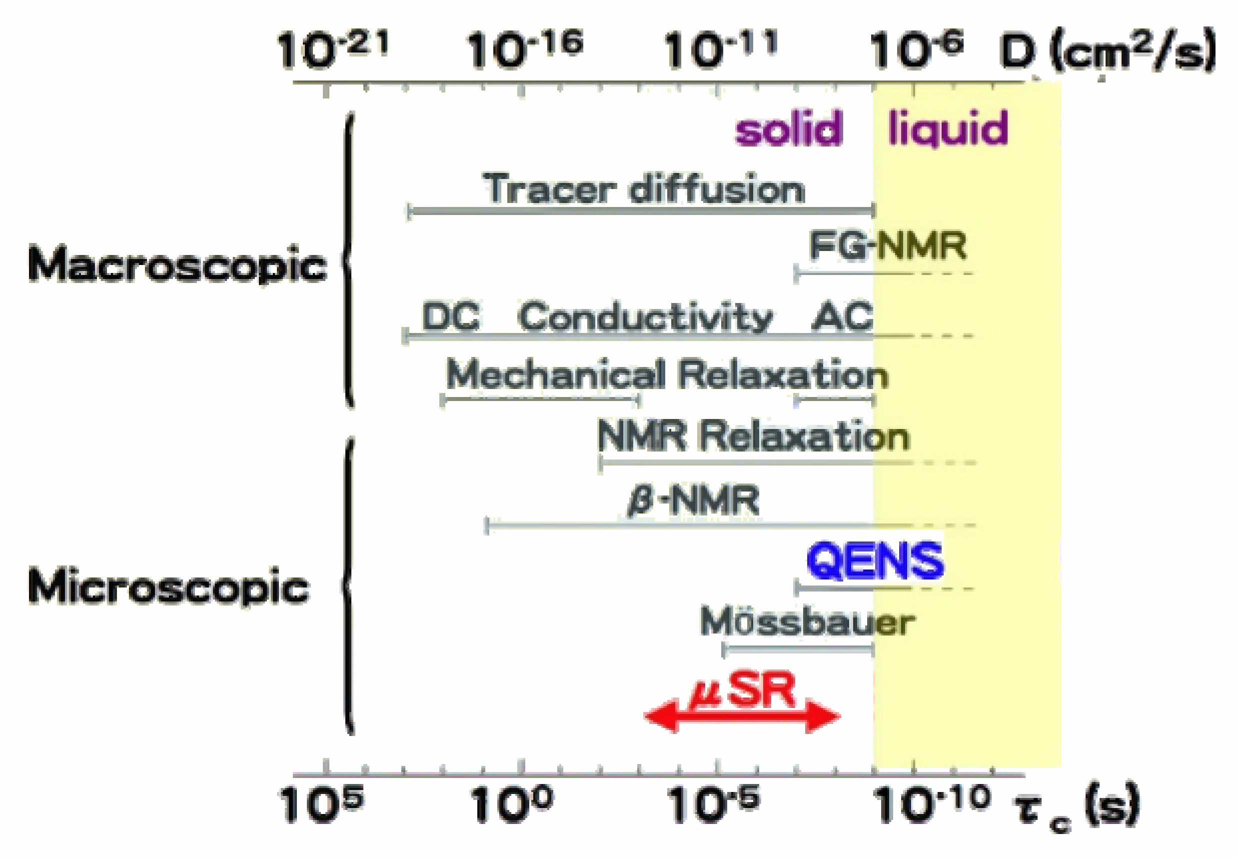
- Could the nano-structuring of a material also be related to the effect we see in pressurized/strained materials ???



Sugiyama, Mansson et al. Phys. Rev. B 92, 014417 (2015)

Summary

- Neutrons and muons are powerful techniques for studying true intrinsic energy material properties & devices + *in operando*.
- Complementary to *e.g.* X-ray techniques + neutron possibilities are developing rapidly, especially in Sweden / at ESS
- Cover different lenght- and time-/energy-scales
- Combined techniques are very powerful but overlapping expertise is rare, let us know if you need help!

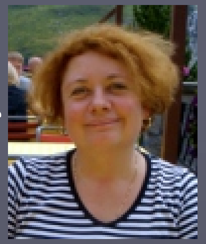


SUSTAINABLE MATERIALS RESEARCH
SMaRT
& TECHNOLOGIES

KTH VETENSKAP OCH KONST

Acknowledgements

Dr. M. Medarde

Dr. E. Pomjakushina

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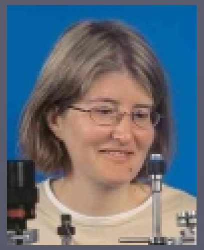
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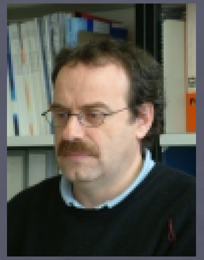
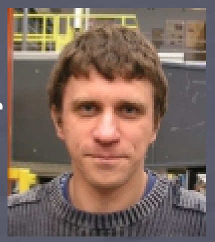
Dr. A. Amato

Dr. A. Suter

Dr. V. Pomjakushin

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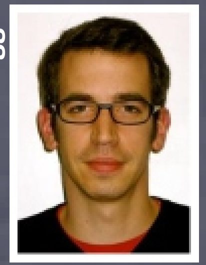

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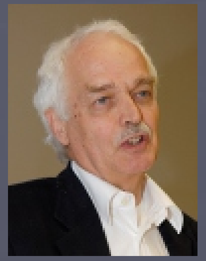
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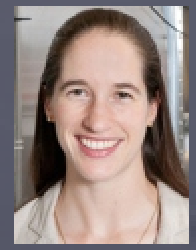
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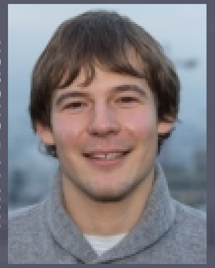
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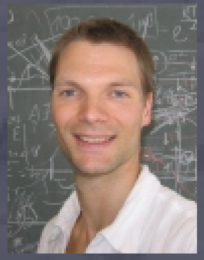

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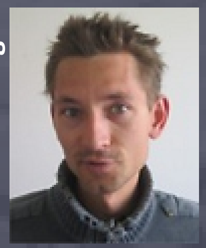

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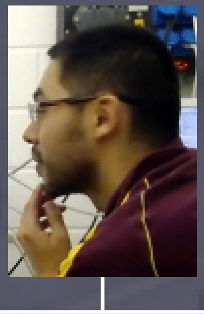
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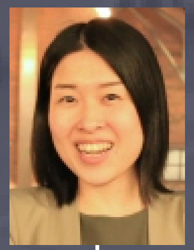

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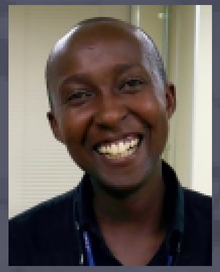

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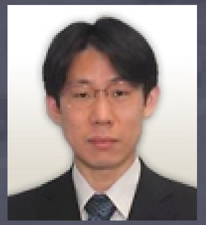
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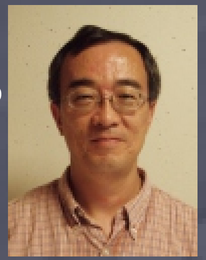
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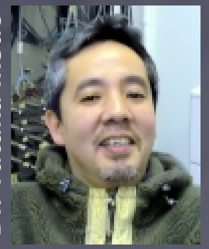
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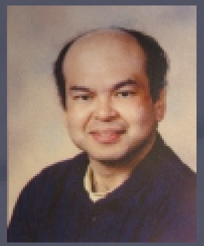
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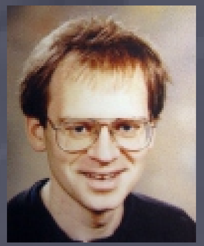
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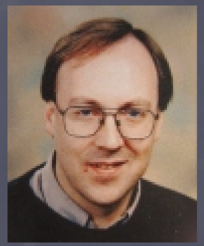
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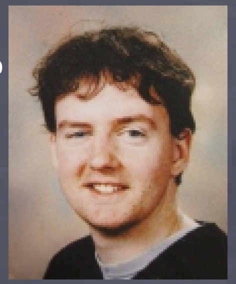

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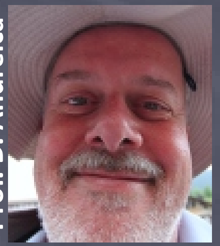

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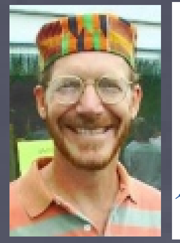

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