LEAPS League of European Accelerator-based Photon Sources

The Battery Challenge

LEAPS Position paper for the European Battery 2030+ Roadmap

The societal challenge

In a world of climate change, energy storage and distribution in form of electrical power are a key challenge to be addressed and tackled in the ambitious **transition of our societies towards fossil-free energy supplies**. Batteries have been identified as one of the major technological challenge in the next decade as they are the core devices to make more efficient use of green energy. **Next generation energy storage** must be based on a diversity of chemistries and architectures that allow batteries to be tailored for specific applications[1,2]. In turn, the **knowledge-based research** on new and **better battery systems** is of fundamental and strategic importance for Europe and the whole world. This research is going to be driven by the ultimate goal to achieve mass production of battery devices adapted to transport, urban and countryside living models, industrial value chain and services to the citizens including healthcare and aging society.

The new challenges for science and engineering

The **target of any rational design of batteries** aims at the control of the migration of electrons, atoms and ions through highly complex and dynamic chemical environments, as well as at the **detailed molecular understanding** of the chemistry and structure of the battery materials. In other words, to achieve **efficiency, reliability, and resiliency** in energy storage technologies a disruptive new level of understanding and control of the local structures and dynamics that determine the electrochemical processes in the battery architecture has to be reached.

We thus ought to understand (see Fig.1)

which processes define the performance of a battery, from the fundamental electro-chemical processes occurring on the nanometer and femtosecond scales to cooperative phenomena within the complex battery architecture on the meso- to micro-length scales and mesoscopic time scales, respectively.

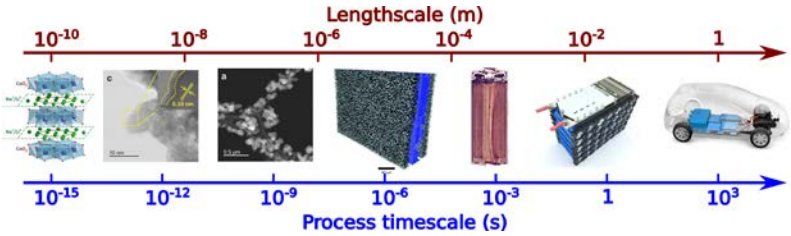

Fig.1 Length scale challenge in future battery research (courtesy: ESRF)

Today, we have only a brittle understanding of the role that **particle size and morphology**, **interface structures and chemistry** play in controlling battery performance. We have no sufficiently detailed information on how **reaction fronts** move through liquids and solids and how this varies with temperature and overpotential.

The key tasks in future battery research projects must thus include (see also Fig.1)

- **correlating** complex electronic, electrochemical and physical **phenomena across all relevant length and time scales,** from sub-micrometer to millimeter and from femtoseconds to hours,
- **understanding** and **controlling** the complex interphase regions formed at **dynamic interfaces**,
- **achieving** better energy storage performance through **novel assemblies of matter**[3], and
- **devising self-healing structures** and **mitigating detrimental chemistries** for longer lifetime and improved safety.

The rational design of future batteries

To address this challenge, battery **processing**, **theory and simulation** and **advanced characterization** must play together in a new way (Fig.2):

Processing

In this new **pan-European effort** candidate materials and assemblies must be prepared with a multitude of growth and preparation parameters which are continuously varied within sensible intervals, in particular regarding stoichiometry, preparation paths and procedures, temperature, pressure, environment gas, liquids and substrates.

Novel processing strategies are mandatory, where a large number of samples are efficiently produced, following **high-throughput pipelines** driven by theoretical prediction, simulation and characterization studies. The success relies in confederating and strengthening European sample processing capabilities involving **industrial stakeholders**.

Theoretical understanding and simulation

Modelling tools spanning first-principles atomistic to phenomenological mesoscale and continuum levels play increasingly important roles in energy storage research. In future, **machine learning strategies** will underpin the data characterizing samples produced through the processing effort and will be the basis for a new approach to penetrate the **complex relationship between function, performance and failure** (affecting energy storage and transport efficiency, reliability, durability, manufacturing complexity and cost, material availability etc.) and the real structure from the atomic scale and characteristic microstructure to typically micron sized assemblies co-existing in mm^3 volumes. To this

purpose, powerful **high throughput computational methods** need to be established, which can receive critical input from sample characterization and provide input to new optimized processing strategies in the theoretical understanding and simulation pipeline. Also here the success relies in confederating and strengthening European simulation and high-power computing availability and access.

Advanced Characterization

Advanced analytical tools encompassing **space- and time-resolved spectroscopy, scattering, imaging, tomography** have seen tremendous advances in the last decade and are key for future energy storage research.

In order to make a critical impact onto rational battery design, thousands of different samples, often made of minute amounts of material (fractions of cubic millimeters), need to be characterized structurally and spectroscopically with real-space resolution, ranging from few-atoms size to sub-micron level. This characterization will require to be carried out under **real operando** conditions, with a hierarchy of different real-space resolution combined -as required- with **element-specific spectroscopy, diffraction, imaging and tomography** strategies, achieving chemical and interatomic resolution. For each sample a rigorous analytical protocol has to be followed zooming from atom to defects, stress development, impurities accumulation, crack development and propagation. This characterization program requires **closest collaboration with processing laboratories**, in order to provide the critical data required to advance our theoretical understanding and underpin simulation studies. The success of this effort relies in confederating and strengthening European characterization capabilities.

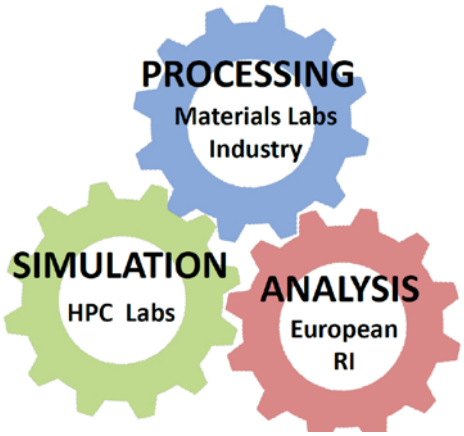

Fig. 2 European Strategy for future Battery Research

The role of LEAPS in a pan-European effort

The modern x-ray facilities of the European LEAPS consortium are poised to meet these demanding analytical challenges.

During the last 20 years, the accelerator-based photon sources, i.e. Synchrotron and Free Electron Laser X-ray facilities, have developed in a spectacular manner and are today a critical link in the materials discovery and innovation chain. In 2017 they all joined forces within the **new European consortium LEAPS**[4]. Its facilities deliver today X-rays a la carte to a multidisciplinary **European scientific community of more than 24.000 scientists** encompassing physicists, chemists, biologists, materials scientists, as well as experts from

medicine, geology and cultural heritage. Furthermore, these facilities provide dedicated experimental environments allowing to carry out operando studies of new materials under all relevant conditions.

LEAPS X-ray facilities provide the **most powerful and unique platforms worldwide** to address all major challenges of the battery characterization aspects. With their highly focused and coherent X-ray beams they simultaneously allow to characterize minute amounts of materials (sub-millimeter level) which can be penetrated and 3-D imaged with real-space resolution ranging from the nanometer to the sub-micron levels. The available and planned X-ray source brilliances and intensities enables high-throughput and time-resolved spectroscopic images at time resolution continuously varying from the femtosecond to the macroscopic second time-scales.

This strength of X-rays is unequalled by other characterization tools which, however, contribute highly relevant complementary information and thus should be included in this pan-European effort. Consequently, **confederating and strengthening European characterization capabilities** should start from an adapted inclusion of existing and planned analytical characterization infrastructures, with a very special role to be provided by the LEAPS facilities as the analytical bedrock for future battery research.

Conclusion

LEAPS proposes a new handshake between the European processing laboratories, the European high performance computing centers and the European analytical facilities to achieve **new levels of electrochemical performance** for next generation batteries. This should be coordinated in an **open innovation** effort involving key European industrial stakeholders to **strengthen industrial leadership** through **accelerated research and innovation** in a global race.

The LEAPS Consortium thus strongly supports the **"BATTERY 2030+"-Roadmap** and **is prepared to play its role** in this **pan-European effort** to devise tomorrow´s batteries.

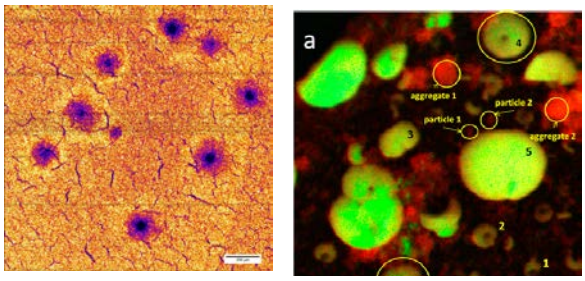

Fig. 3 Synchrotron X-ray studies of Li battery materials

(left) X-ray micro-tomography of the manganese distribution (purple) in a $LiNi_{0.5}Mn_{1.5}O_4$ electrode after 25 fast charging cycles (courtesy: DESY)

(right) X-ray Transmission microscopy image of the discharge products in ether-based LiO_2 cells cyan: Li superoxide, green: Li peroxide, red: carbonate (courtesy: ALBA).

References

1/ DOE: Basic Research Needs for Next Gen Electrical Energy Storage (2017)
2/ EC – Batstorm: Support to R&D Strategy for battery based energy storage (2016)
3/ J. Power Sources 382, 176 (2018)
4/ LEAPS Consortium: https://leaps-initiative.eu/