LENS LEAGUE OF ADVANCED EUROPEAN NEUTRON SOURCES

LENS Position Paper on "BATTERY 2030+ Roadmap (Second Draft)"

As the BATTERY 2030+ Roadmap makes abundantly clear, the strategic use of large-scale European analytical facilities will play a critical role in realising the roadmap and especially the Battery Interface/Interphase Genome and Materials Acceleration Platform (BIG-MAP) research area. The neutron and photon facilities represented by the pan-European LENS and LEAPS initiatives are specifically singled out in this respect. With this paper, LENS wishes to clearly support the proposed strategy in a manner that is consistent with and builds upon a complementary paper to be submitted by the light source initiative, LEAPS.

LENS feels that the references made to neutron-based experimental techniques in the BATTERY 2030+ Roadmap could usefully be made even stronger by isolating three areas of contribution that neutron sources will make to this mission-based project. Once these areas are clearly identified as foundational, the specific actions, time scales and funding mechanisms necessary to enable facility contributions will begin to emerge as essential Roadmap milestones.

LENS facilities are important contributors to the BATTERY 2030+ Roadmap early on, where BATTERY 2030+'s success in implementing BIG-MAP will determine the pace for the European Battery Alliance, Batteries Europe and BATTERY 2030+ project as a whole. We feel the fundamental role of Europe's large-scale photon and neutron sources could helpfully be made more explicit in the Roadmap, as the efficient use of these facilities requires careful advance planning.

The 10-year plan for BATTERY 2030+ must rely heavily on infrastructures either already in operation or coming into operation during the next decade. Success relies on identifying from the start how the development and use of specific capabilities, instruments and access protocols needs to be coordinated to support the BATTERY 2030+ mission. This sort of coordination is precisely the role of the LENS initiative, and thus these activities are very much already in motion. But their specific interface with BATTERY 2030+ must be more clearly defined.

LENS therefore recommends that the Roadmap highlight the following three areas of mission-oriented contributions to be made by LENS facilities to the BATTERY 2030+ roadmap:

- Investment in the development of new or upgraded **instrumentation** that will enable the *in situ* and *in operando*, multi-length-scale X-ray and neutron experimental techniques and methodologies necessary for rapid development of better batteries;
- The accelerated development and standardisation of open-source neutron **data management protocols and data analysis software**, along with that of the **shared infrastructure** necessary to extract rapidly the unique information content from the data sets produced at Europe's large-scale facilities;
- The establishment of access channels on those European large-scale facilities that can provide neutron instrumentation best suited to BATTERY 2030+'s research needs during each stage of the project.

Development of advanced instrumentation

The viability of the BATTERY 2030+ project relies on early-stage efforts to establish workflows for both in-depth and high-throughput testing of materials and chemistries, research methodologies that, among other needs, will require the most advanced neutron instrumentation and technologies. These systems will necessarily need to be designed, constructed and operated at high-flux large-scale facilities. The

current state-of-the-art is not sufficient for what is envisioned during the full operational mode of the BATTERY 2030+ Roadmap, as it will require orders of magnitude increases in the speed of measurement, measurement across length scales from the atomic scale to the micron scale, and an accompanying advancement of methodologies. This can only be achieved through additional investment in close coordination with the facilities and researchers represented by LENS. Given the long lead-times associated with developing instruments and instrument technologies, the actions related to advanced instrumentation must be defined at a very early stage of the roadmap.

Data management, analysis and infrastructure

The other side of the accelerated development of inversely engineered battery designs is BATTERY 2030+'s exploitation of large curated data sets and the e-infrastructures that can support them. Europe's large-scale neutron sources are uniquely positioned not only to generate such data sets but also to provide the competencies required to expand and exploit them. Among LENS (and LEAPS) facilities, several initiatives are already in progress that aim to standardise the management and accessibility of scientific data and data analysis software, as well as to establish shared infrastructures. These include PaNOSC, ExPaNDs and many other activities feeding into the realisation of FAIR data principles for photon and neutron scattering data within the framework of the European Open Science Cloud. Furthermore, on account of the large curated data sets managed by neutron and photon sources, LENS facilities are active in other initiatives targeting the advancement of machine learning and the application of AI to scientific investigations.

Access to beam time

Serving a community of more than 5,000 users, beam time at Europe's neutron sources is severely oversubscribed by a factor of more than two, and demand is increasing. In the case of neutron sources, capacity (as measured in instrument-days) dropped by 17% with the closures of three reactor sources in 2019. The European Spallation Source will come online with three neutron instruments in 2023, but will require nearly a decade more to reach full capacity. It is therefore of utmost importance to the BATTERY 2030+ Roadmap that it develops access channels for beam time at both existing and emerging facilities required during different stages of the project. This will require careful advance planning that will naturally go hand-in-hand with the development of the advanced instrumentation described above.

Europe is extremely well positioned in this respect. It provides a world-leading suite of highly complementary facilities, where the fastest measurements can be made. All of these facilities have strong existing links to the scientific community working on the various aspects of battery development. This has allowed scientists working at Europe's neutron sources to gather tremendous prior competence in the field. Upgrades at all major sources are underway and the world's most powerful neutron source, ESS, will begin user operations in 2023.

This is an ideal moment to realize the specific requirements of the BATTERY 2030+ initiative in a timely manner. LENS very much looks forward to working closely with BATTERY 2030+ to further develop specific actions to achieve the ambitious and highly valuable potential of this pan-European research and innovation effort.