D1.11 – Proceeding from international workshop/conference

VERSION

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ABSTRACT

Today, energy production and transport are evolving fast to meet challenging environmental targets and growing demand. The Achilles' heel is energy storage, which is incapable of providing both low-cost and high-performance solutions. The answer is not a simple evolution of existing batteries but disruptive technologies that must be discovered fast. The BIG-MAP vision is to develop a modular, closed-loop infrastructure and methodology to bridge physical insights and data-driven approaches to accelerate the discovery of sustainable battery chemistries and technologies. BIG-MAP's strategy is to integrate machine learning, computer simulations cohesively, and AI-orchestrated experiments and synthesis to accelerate battery materials discovery and optimization. The project will be a lever to create the infrastructural backbone of a versatile and chemistry-neutral European Materials Acceleration Platform, capable of reaching a 10-fold increase in the rate of discovery of novel battery materials and interfaces.

This deliverable, included in the WP 1 'Project management, education, exploitation and outreach', aims at reporting on international workshops and/or conferences (co)-hosted together with the other LC-BAT-2020 consortia. In this regard, in 2021, BIG-MAP joined, together with other LC-BAT-2020 projects, two main international conferences that brought high visibility among the battery research and innovation community: The BATTERY 2030+ Annual Conference that took place on October 7, 2021 (see chapter 1) and the Battery Innovation Days (BID), held on 23-25 November 2021 (see chapter 2).

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1. BATTERY 2030+ Annual Conference

1.1 Introduction

The Annual Conference of the BATTERY 2030+ entitled 'Empowering Green Innovation' was held online on October 7th, 2021, from 9.30h to 16.30h. Gathering all organisations directly involved in the BATTERY 2030+ CSA and in one of the projects of the LC-BAT-2020, the BATTERY 2030+ Annual Conference was recognized as a Sustainable Energy Day, an online side event of the EU Sustainable Energy Week (EUSEW 2021).

The main objective of the conference was to exchange knowledge on the BATTERY 2030+ roadmap update and on the preliminary results already achieved by the projects of the LC-BAT-2020 programme falling under the umbrella of BATTERY 2030+, with a particular emphasis on scientific aspects.

2.1 Programme and attendance

Apart from the presentations of the preliminary results already achieved by all the LC-BAT-2020 projects, the Annual Conference included guest speakers from the European Commission - DG-CNECT and EBA250. Furthermore, the Annual Conference inaugurated the BATTERY 2030+ Excellence Seminars: a series of seminars where top speakers are invited to give keynote presentations about batteries. Figure 1 below shows the programme of the Annual Conference.

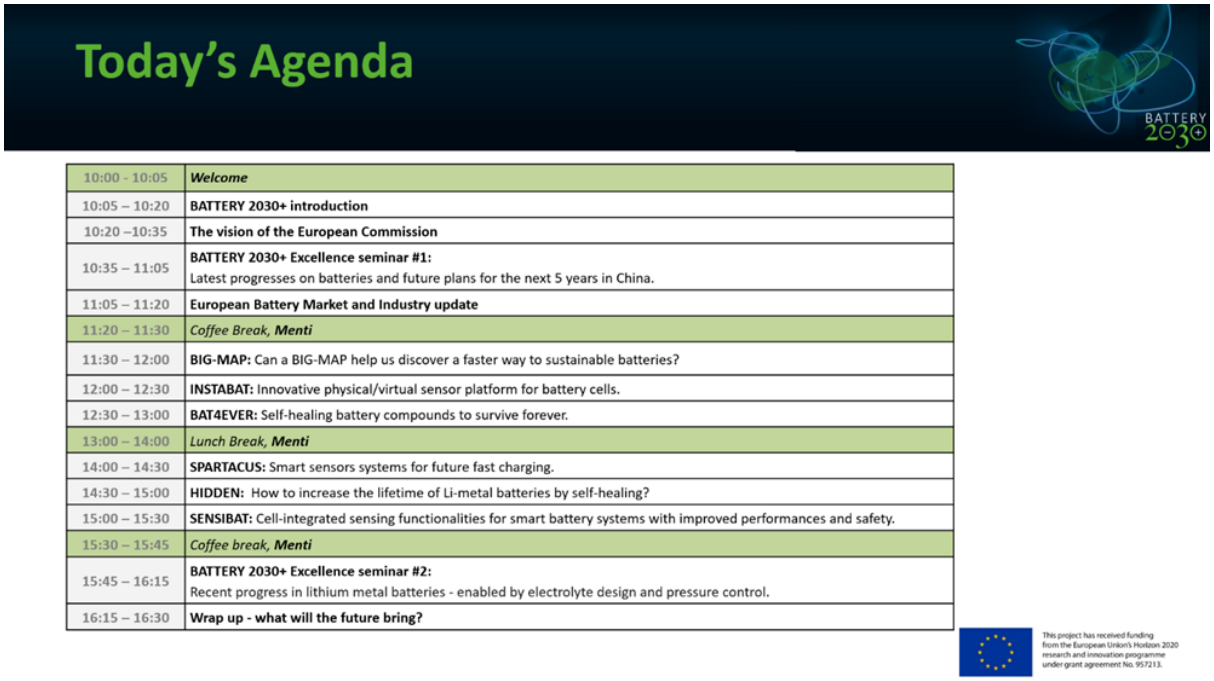


Figure 1. BATTERY 2030+ Annual Conference Programme

A total of 587 participants registered for the BATTERY 2030+ Annual Conference. It is very difficult to provide the exact number of participants who joined all or part of the conference, but at least a peak of 264 participants connected at the same time were counted. As the graphics Figure 2 shows, 57 % of the registrations came from research organisations, followed by 24 % of participants from industry. Regarding the origin country of the participant organisations, we see a very split graph with registrations mostly coming from all over Europe but also from other regions such as the USA, China, India, and Pakistan (Figure 3).

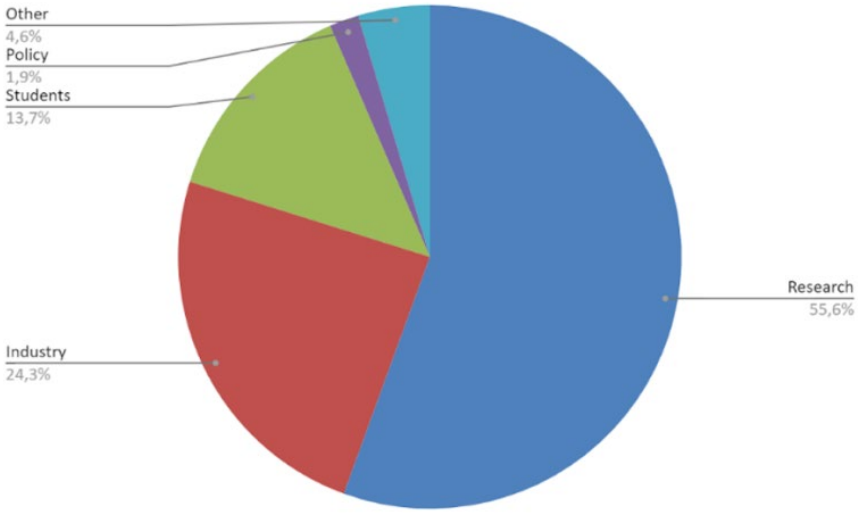


Figure 2. Registration by organization type

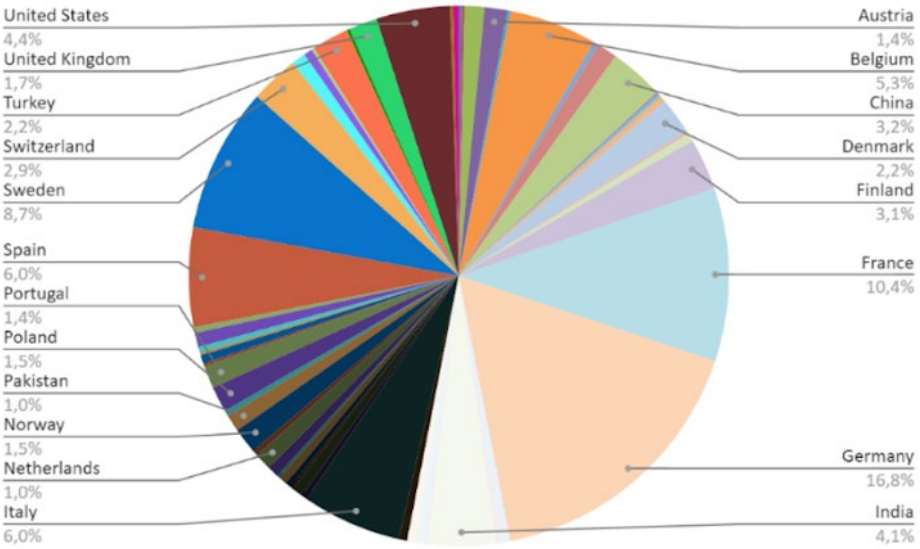


Figure 3. Registration by country

3.1 Content of BIG-MAP presentation

The session 'Can a BIG-MAP help us discover a faster way to sustainable batteries? was presented by Prof. Tejs Vegge, the BIG-MAP project coordinator. The presentation addressed all the following topics:

- Accelerated battery discovery infrastructure
- Digitalizing the battery discovery process
- Chemistry agnostic uncertainty-aware ML for early prediction of battery degradation
- Shared data infrastructure and interoperability
- Battery Interface Ontology (BattINFO)
- An operation data management plan
- Operational DPM: from words to code
- BIG-MAP App store and Github repository
- Electronic BIG-MAP logbook
- Electrochemical data and metadata exchange
- PRISMA: Phyton-based, Robust, data-Intensive Spectrum Monitoring App
- Integrated autonomous discovery workflows
- Autonomous workflows for thermodynamic and kinetic properties
- Understanding and controlling interfaces
- NPPs for battery electrolytes and interfaces
- D2.1 Initial QM databases for ML-training and analysis
- BIG-MAP as a LUMI pilot project
- Multi-domain, multi-fidelity data, and models
- D11.1 Initial model for dynamic fidelity assignment
- Identifying Dynamic Deep Interface Descriptors
- Deep descriptors & XAI for battery interfaces
- BATTERY 2030+ joint undertakings: ontology compliant DMPs across projects
- Operando characterization of smart batteries: BIG-MAP + INSTABAT collaboration

To wrap up the BIG-MAP session, Prof. Vegge concluded the presentation with a brief summary and next steps:

- BIG-MAP: transitioning from sequential and Edisonian battery development to autonomous discovery of battery materials and interfaces/interphases
- Developing AI-orchestrated acquisition of multi-domain and multi-fidelity data discovery and synthesis process
- Furthering the common battery ontology (BattINFO), standards and protocols
- Develop dynamic data management plans and a shared data-infrastructure for FAIR data with externalizable tools (BIG-MAP GitHub repository and app store)
- Creating closed-loop discovery workflows bridging simulations and experiments using uncertainty quantification.
- Developing physics-aware and spatio-temporal deep learning and XAI models for inverse design of battery materials and interfaces.

The slides of the BIG-MAP presentation are attached as **Annex 1**.

2. Battery Innovation Days (BID)

2.1 Introduction

The 1st edition of the Battery Innovation Days (BIDs), the annual conference on battery research and innovation, took place online on 23-24-25 November 2021. Co-organised by the most important European initiatives coordinating R&I activities (the BATTERY 2030+ initiative, the ETIP BATTERIES EUROPE, the Batteries European Partnership Association (BEPA) and the 1st and 2nd IPCEIs on Batteries), the event was designed to bring together numerous key players and experts from the battery R&I field, including representatives from the European Commission.

The Battery Innovation Days' main goal is to annually gather the whole European battery community active in research and innovation. The event is an opportunity for industry leaders to converge and provide hot takes on the latest developments within the European R&I Battery domain, exchange views on key strategic approaches to deploying crucial technologies, and assess future R&I needs for a more competitive and sustainable European battery value chain.

2.2 Programme and attendance

The Battery Innovation Days offered 2.5 days of keynote presentations and breakouts sessions to discuss research and innovation within the field of batteries. Besides the talks, plenty of additional side activities were available during and after the event, such as the Exhibitor Area available to collaborative projects to showcase their results, the Battery Young Research Awards, and the Networking Area. BIG-MAP was one of the 27 projects and initiatives exhibiting during this event.

Below is a summary of each day:

- During Day 1, attendees discovered the different bodies supporting the development and deployment of a competitive and sustainable battery value chain at the European level and gained a better understanding of the current status of the battery market worldwide, what the long-term priorities are, and why circularity and safety are of the essence.

- During Day 2, attendees gained insights on the sustainability status of the battery value chain, discovered the future disruptive technologies that will revolutionize the field, what research is being carried out to support a competitive automotive industry, and smart battery functionalisation. The Battery Young Research Award was delivered in the afternoon of the second day.

- During Day 3 attendees dived into Future R&I priorities for 2023-2024, and learnt more about new emerging markets, the importance of digitalization, and the necessity to train students and workers who can support the European industry.

For more detail, see the full agenda in **Annex 2**.

More than 2000 people from all over the world registered at the Battery Innovation Days, and 1521 attended at least one session. The graph below illustrates a dominant presence of participants from all over Europe, but also Australia, the USA and some Asian countries are represented (Figure 4).

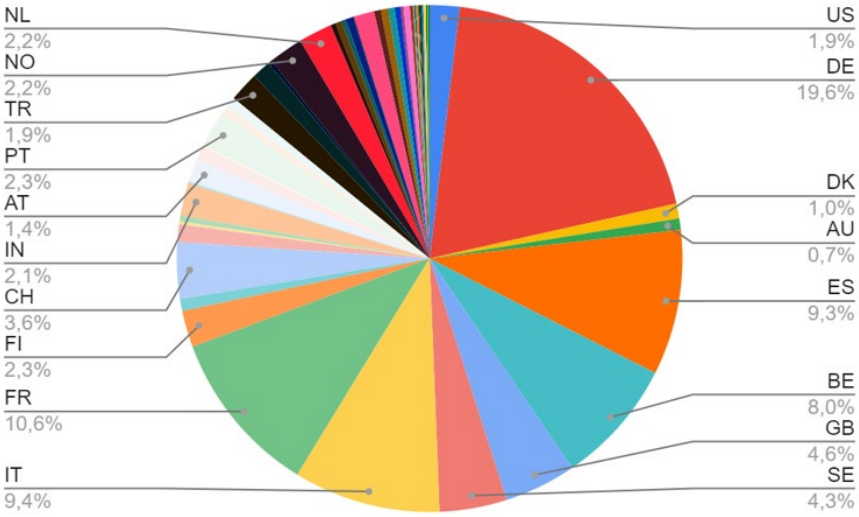


Figure 4. Registration by country

2.3 BIG-MAP participation

During the Battery Innovation Days, BIG-MAP gained high visibility by actively participating in the two sessions presented below. Furthermore, BIG-MAP was represented in the Exhibition Area in the BATTERY 2030+ booth and the BIG-MAP own booth, which contained information about the project, an introductory video and the website.

- **Nov. 23 (2-3:30 PM) - Long-term research for batteries: what are the next priorities?**

BATTERY 2030+ has been working on long-term research priorities for four years. In this session, players from the industry and research area discussed the priorities that need to be set now for Europe to remain competitive and sustainable looking beyond 2030.

The session opened with a presentation on Long-term European roadmaps for battery research. Following, there was a panel discussion on what battery chemistries we can hope for in the future to benefit European industry. A second panel discussion explored 'how we can enable the chemistries of the future', where BIG-MAP played a key role.

- **Nov 25 (9.30-11 AM) - From raw materials to applications: the indispensable necessity of digital development**

Digitalization is of the essence to decarbonise the economy. This session aimed at showing the importance of digitalization along the value chain and its role in the acceleration of R&I on battery materials and cells. The session opened with a presentation focused on how digitalisation is now the prerequisite to developing a green value chain. Following, a panel discussion explored HE Partnerships and digital innovations along the value chain. The session ended with a second panel discussion on how digitalisation is accelerating R&D on battery materials and cells. This second panel discussion was a perfect opportunity for Prof. Tejs Vegge to introduce BIG-MAP and BATTERY 2030+ and demonstrate their relevance.

Some of the topics covered by the coordinator of BIG-MAP during these two sessions of the Battery Innovation Days are listed below:

- Transcending Edisonian Battery Development
- Modular Materials Acceleration Platform
- Accelerated battery discovery infrastructure
- Autonomous discovery workflows

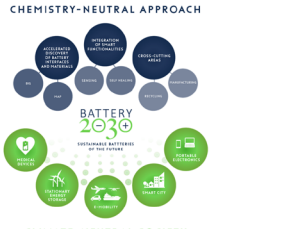
3. Conclusion

One of the main objectives of the BIG-MAP WP1 'Project management, education, exploitation, and outreach' is to enable close contact with a broad network of stakeholders by taking part in networking events/conferences and by arranging project events like stakeholder meetings, seminars, and workshop/conferences. By participating in the Battery 2030+ Annual Conference and the Battery Innovation Days, BIG-MAP has gained high visibility and reputation among the European battery research and innovation ecosystem and highlighted the identified synergies with other LC-BAT-2020 projects.

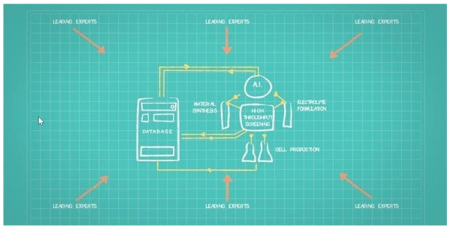
Annex 1 – BIG-MAP presentation at the BATTERY 2030+ annual conference

BIG-MAP: Battery Interface Genome - Materials Acceleration Platform

BATTERY 2030+ annual meeting – Empowering Green Innovation



Can a BIG-MAP help us discover a faster way to sustainable batteries?



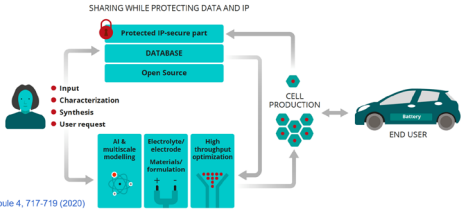
Brenville, Palacin, Christensen, BIG-MAP (2021)

Welcoming BIG-MAP to Copenhagen!

- BIG-MAP project meeting on September 17th with 90 live and 40 Zoom participants
- Great to finally meet face-to-face!

Accelerated battery discovery infrastructure

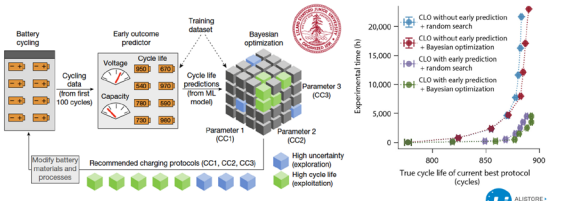
- Accelerated closed-loop discovery using AI-accelerated models & procedures
- Toward smarter batteries with AI and multisensory and self-healing approaches



Bhowmik, Vegge, Joule 4, 717-719 (2020)
Vegge, Tarascon, Edström, Adv. Energy Mater. 11, 2100362 (2021); Cekic-Laskovic, Stein, Grimaud, et al. (2021)

Digitalizing the battery discovery process

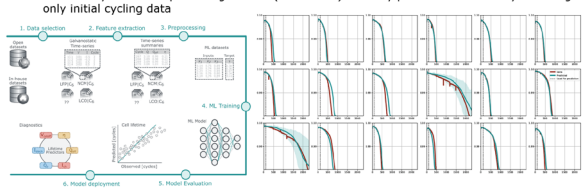
- State-of-the-art: ML-assisted digital optimization of battery performance and utilization
- Next step: AI-assisted development of new insights into the limiting processes



Attia, Chueh et al., Nature 578, 397–402 (2020); Bhowmik, Vegge, Joule 4, 717-719 (2020)
Lombardo, Bhowmik, Ayerbe, Grimaud, Vegge, Johansson, Franco, et al., Chem. Rev. 10.1021/acs.chemrev.1c00108 (2021)

Chemistry agnostic uncertainty-aware ML for early prediction of battery degradation

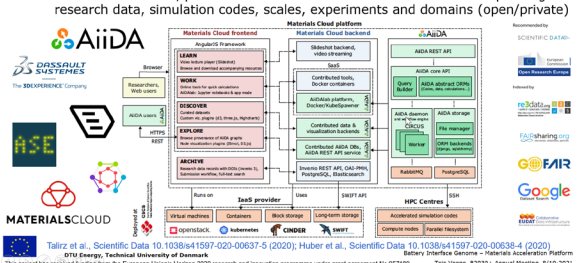
- Can deep learning accelerate the discovery process by providing new insights?
- Uncertainty-aware deep learning models (LSTM-RNN) for early predictions of battery life using only initial cycling data



Busk, Jørgensen, Bhowmik, Schmidt, Winther, Vegge, arXiv:2107.06068 (2021)
Rieger, Flores, Nielsen, Norby, Ayerbe, Winther, Vegge, Bhowmik, *Uncertainty-aware and explainable machine learning for early prediction of battery cell degradation*, arXiv (2021)

Shared data infrastructure & interoperability

- Focus on standards, protocols and a shared FAIR data-infrastructure spanning research data, simulation codes, scales, experiments and domains (open/private)



Talirz et al., Scientific Data 10.1038/s41597-020-00637-5 (2020); Huber et al., Scientific Data 10.1038/s41597-020-00638-4 (2020)

Battery Interface Ontology (BattINFO)

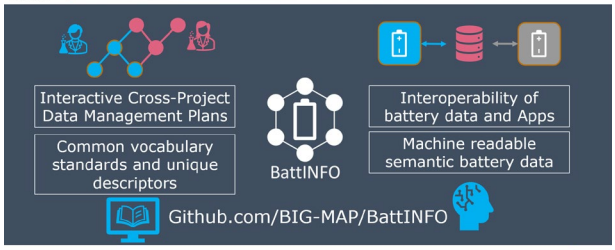
The **Battery Interface Ontology** is a formal, **machine-readable model** encapsulating **knowledge** about **electrochemistry** and **batteries**.

BattINFO

Based on the top-level Elementary Multiperspective Materials Ontology (EMMO)

Clark, Friis, et al. (2021)

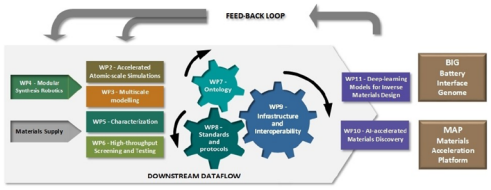
Battery Interface Ontology (BattINFO)



Clark, Friis, et al. (2021)

An operational data management plan

- A "living" data management and data exchange/utilization plan is needed



Castelli et al, Batteries & Supercaps 4, 1-11 (2021)

DTU Energy, Technical University of Denmark

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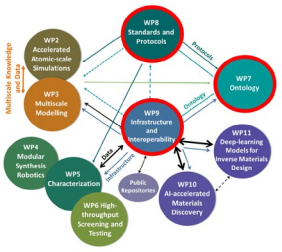
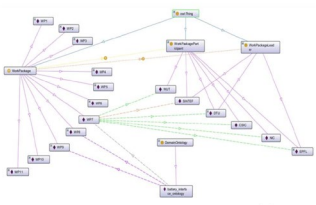
Battery Interface Genome – Materials Acceleration Platform

Tejs Vegge, B2030+ Annual Meeting, 8/10-2021

Operational DMP: from words to code



Include ontology concepts into the BIG-MAP DMP



Courtesy Simon Clark

Castelli et al, Batteries & Supercaps 4, 1-11 (2021)

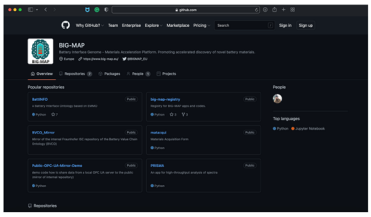
DTU Energy, Technical University of Denmark

Battery Interface Genome – Materials Acceleration Platform

Tejs Vegge, B2030+ Annual Meeting, 8/10-2021

BIG-MAP App store and GitHub repository

- Developing externalizable tools, apps and workflows for the European battery community
- We've created a GitHub BIG-MAP repository and a BIG-MAP app store



Pizzi, Marzari, Wenzel, et al. (2021)

DTU Energy, Technical University of Denmark

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Battery Interface Genome – Materials Acceleration Platform

Tejs Vegge, B2030+ Annual Meeting, 8/10-2021

Electronic BIG-MAP logbook

- Providing a mechanism to locate, organize and "put in context" the data produced within the BIG-MAP project in order to foster collaboration

Caro, Flores, Grimaud, Franco (2021)

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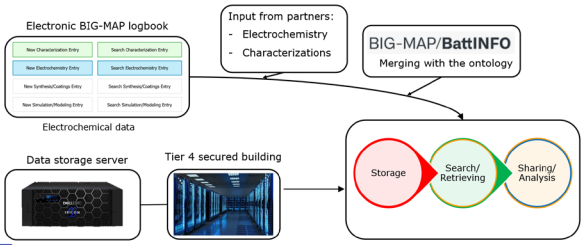
Electrochemical data and metadata exchange



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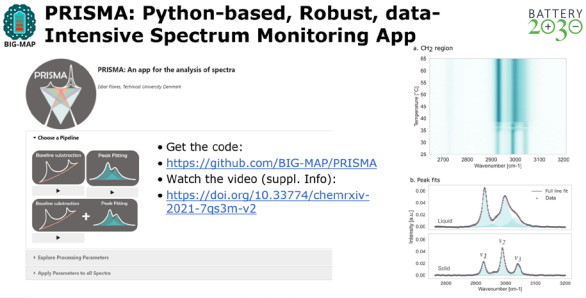
Battery Interface Genome – Materials Acceleration Platform

Tejs Vegge, B2030+ Annual Meeting, 8/10-2021

PRISMA: Python-based, Robust, data-Intensive Spectrum Monitoring App



- Get the code:
- https://github.com/BIG-MAP/PRISMA
- Watch the video (suppl. Info):
- https://doi.org/10.33774/chemrxiv-2021-7qs3m-v2

Flores, Mozhzhukhina, Li, Norby, Matic, Vegge, ChemRxiv 10.33774/chemrxiv-2021-7qs3m-v2 (2021)

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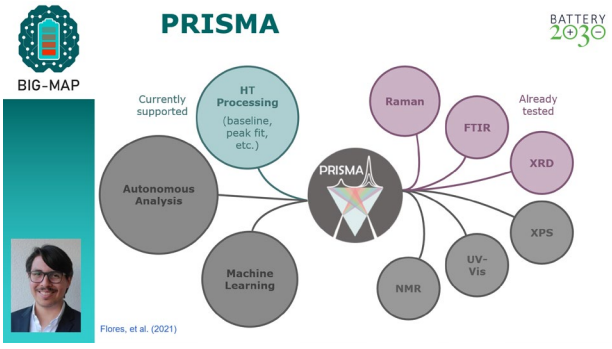
Battery Interface Genome – Materials Acceleration Platform

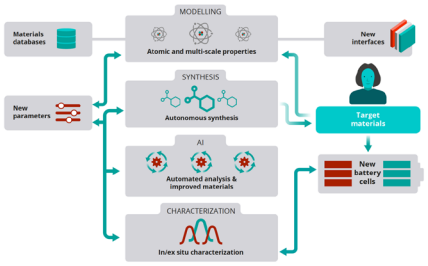
Tejs Vegge, B2030+ Annual Meeting, 8/10-2021

PRISMA



Flores, et al. (2021)

Integrated autonomous discovery workflows



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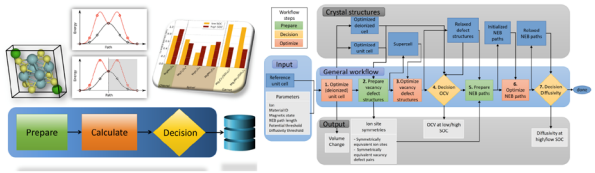
Autonomous workflows for thermodynamic and kinetic properties

- Automated workflows for discovery of new electrode materials
- Fast screening and analysis of ICSD structures for thermodynamic and kinetic properties
- Expedited exploration of crystal structures with distinguishable migration characteristics



Bölle, Mathiesen, Nielsen, Vegge, García-Lastra, Castelli, Batteries & Supercaps 3, 488 (2020)
Bölle, Bhowmik, Vegge, García-Lastra, Castelli, Batteries & Supercaps, 10.1002/batt.202100086 (2021)

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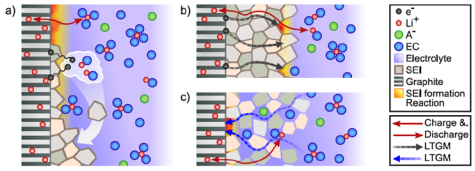
Understanding & controlling interfaces

- Interfaces and interphases play a critical role in all battery technologies
- Physical understanding is essential to develop models for accelerated discovery

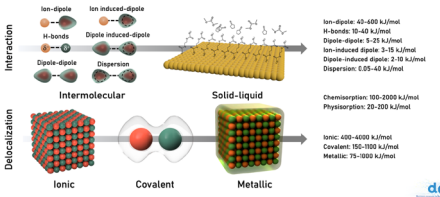


Horstmann, Single, Latz, Current Opinion in Electrochemistry 13, 61-69 (2019)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

NNPs for battery electrolytes and interfaces

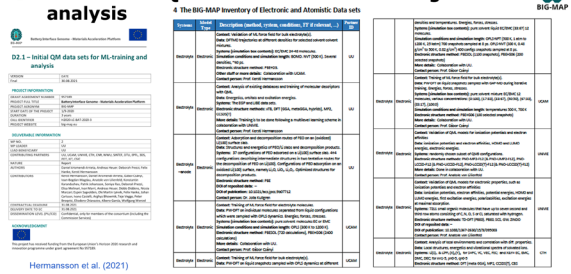
- Developing generalizable workflows for training machine learning potentials for complex systems with large variations in inter- and intra-molecular forces
- The physics at interfaces and the influence of structure/morphology must be well described



Bhowmik, Bereciibar, Casas-Cabanas, Csanyi, Dominko, Hermansson, Palacin, Stein, Vegge (2021)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

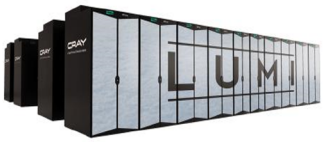
D2.1 Initial QM datasets for ML-training and analysis



Hermansson et al. (2021)

BIG-MAP as a LUMI pilot project

- What's happening in the future?
- BIG-MAP is set to test the new 552 peta flops EuroHPC facility LUMI
- High-fidelity electronic structure data from deep neural networks going beyond variational Quantum Monte Carlo (QMC)
- Hierarchical latent space multi-scale models



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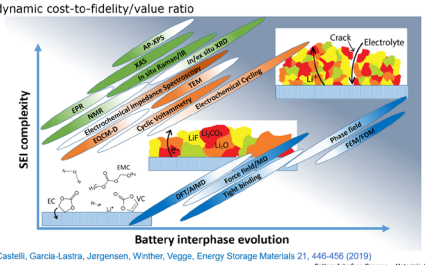
Multi-domain/multi-fidelity data and models

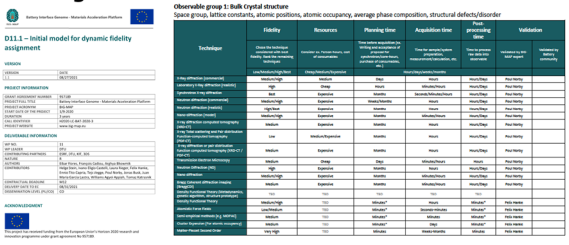
- A dynamic cost-to-fidelity/value ratio



Bhowmik, Castelli, Garcia-Lastra, Jørgensen, Winther, Vegge, Energy Storage Materials 21, 446-456 (2019)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

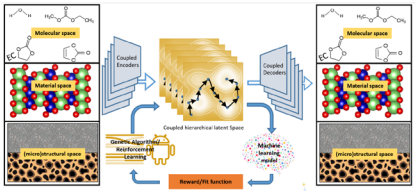
D11.1 Initial model for dynamic fidelity assignment



Capria, Cadiou, Bhowmik, Hanke, Flores, Norby, et al. (2021)

Identifying Dynamic Deep Interface Descriptors

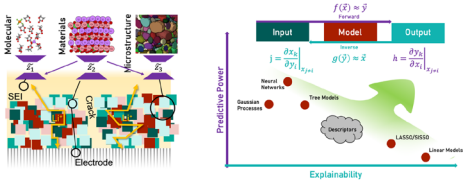
- Inverse design of battery interfaces with spatio-temporal multiscale models
- Generative deep learning to identify dynamic interface descriptors



Bhowmik, Castelli, Garcia-Lastra, Jørgensen, Winther, Vegge, Energy Storage Materials 21, 446-456 (2019)

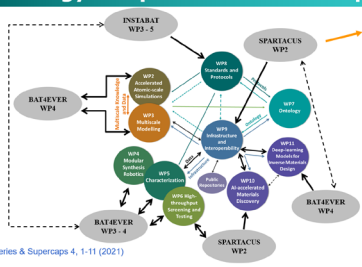
Deep descriptors & XAI for batttery interfaces

- Developing hybrid physics/data-driven and explainable AI (XAI) models for battery interface evolution



Bhowmik, Berecibar, Casas-Cabanas, Csanyi, Dominko, Hermansson, Palacin, Stein, Vegge (2021)

BATTERY 2030+ joint undertakings: Ontology compliant DMPs across projects



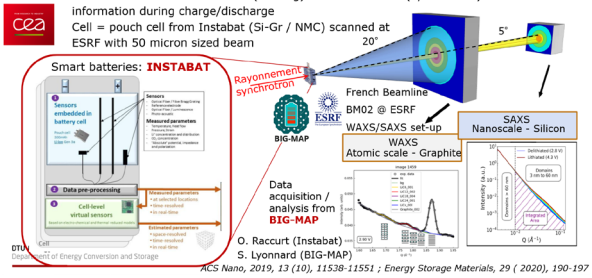
Joint demonstrator to demonstrate sharing and utilization of data:

- Modelling
- Electrochemistry
- Synthesis and testing
- Sensing
- Self-healing

Castelli et al, Batteries & Supercaps 4, 1-11 (2021)

Operando characterization of smart batteries: BIG-MAP + INSTABAT collaboration

Aim: correlate the "macroscale" (sensing) and "microscale" (synchrotron) information during charge/discharge
Cell = pouch cell from Instabat (Si-Gr / NMC) scanned at ESRF with 50 micron sized beam



O. Raccurt (Instabat) — S. Lyonnard (BIG-MAP)

ACS Nano, 2019, 13 (10), 11538-11551 ; Energy Storage Materials, 29 (2020), 190-197

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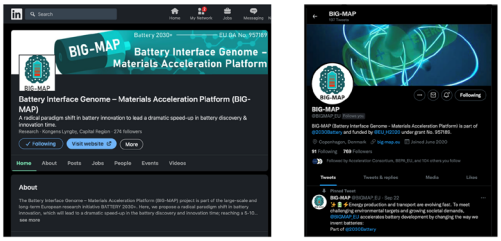

Summary and next steps

- BIG-MAP: transitioning from sequential and Edisonian battery development to autonomous discovery of battery materials and interfaces/interphases
- Developing AI-orchestrated acquisition of multi-domain and multi-fidelity data from simulations, machine learning and experiments to accelerate the discovery and synthesis process
- Furthering the common battery ontology (BattINFO), standards and protocols
- Develop dynamic data management plans and a shared data-infrastructure for FAIR data with externalizable tools (BIG-MAP GitHub repository and app store)
- Creating closed-loop discovery workflows bridging simulations and experiments using uncertainty quantification
- Developing physics-aware and spatio-temporal deep learning and XAI models for inverse design of battery materials and interfaces

Acknowledgment

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Annex 2 - BID agenda

DAY 1: 23rd of November 2021		
9:30-11:30	Plenary 1: Research and Innovation across the European Battery value chain: the need for a comprehensive and complementary approach	
11:30-12:30	Creating a circular European Battery Value chain (Recycling; Second life batteries …)	
12:30-14:00	Lunch Break	
14:00-15:30	Long term research for batteries: what are the next priorities ?	Research and Innovation worldwide, what's going on ?
15:30-16:00	Coffee Break	
16:00-17:00	Further improving batteries safety: What's needed ?	R&I support for the further deployment of stationnary storage

DAY 2: 24th of November 2021		
9:30:-11:30	Plenary 2: A paramount to achieve decarbonization objectives: The further development of sustainable batteries.	
11:30-12:30	Smart battery functinalisation: status and future	Outlook of manufacturing activities along the battery value chain in Europe
12:30-14:00	Lunch Break	
14:00-15:30	Solid-state research, promising future, Next disruptive technologies.	Battery research to support a competitive automotive industry
15:30-16:00	Coffee Break	
16:00-17:00	Battery Young Research Award	

DAY 3: 25th of November 2021		
9:30-11:00	Future R&I priorities for 2023-2024, what's on the table ?	From raw materials to application: the indispensable necessity of digital development
11:00-12:00	Jobs creation and bridging the skills gap across the European battery value chain	New emerging market and applications (Airborne, waterborne, rail, off-road, agriculture)
12:00-12:15	Coffee Break	
12:15-13:15	Plenary 3: Industrial Innovation Uptake: Succeeding on the road from lab to market	