



The BIG-MAP Stakeholder Initiatives



DTU Energy, Technical University of Denmark

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



Why launch the Stakeholder Initiatives (SI)?

BATTERY
2030

- To strengthen the integration of the BIG-MAP infrastructure with leading external stakeholders, widely used soft- and hardware infrastructure and equipment, etc., in the battery community
- The SI projects are smaller, focused collaborative projects between one or more external stakeholders and one or more BIG-MAP partners targeting the integration of the BIG-MAP infrastructure in the European value chain for battery discovery and development
- Why now?
 - We would like our stakeholders and the community to be involved from the start



Call for BIG-MAP Stakeholder Initiatives

The Battery Interface Genome - Materials Acceleration Platform (BIG-MAP) is the largest of the seven H2020 projects constituting the large scale and long term European research initiative BATTERY 2030+ (www.battery2030.eu). BIG-MAP constitutes a joint effort of 34 European partners spanning academia, research organizations and industry (www.big-map.eu) to create a paradigm shift in battery innovation, which will lead to a dramatic acceleration of the battery discovery process, achieving a 5-10-fold increase relative to the current rate of discovery within the next 5-10 years. BIG-MAP relies on the development of a unique R&D infrastructure and accelerated methodology that unites and integrates insights from leading experts, competences and data throughout the battery (discovery) value chain with Artificial Intelligence (AI), high-performance computing (HPC), large-scale and high-throughput characterization and autonomous synthesis robotics. In short, BIG-MAP aims to reinvent the way we invent batteries and to develop core modules and key demonstrators of a Materials Acceleration Platform specifically designed for the accelerated discovery of battery materials and interfaces.

To strengthen the integration of the BIG-MAP infrastructure with leading external stakeholders, widely used soft- and hardware infrastructure and equipment, etc., in the battery community, BIG-MAP launches a call for so-called Stakeholder Initiatives (SI). The SI projects are smaller, focused collaborative projects between one or more external stakeholders and one or more BIG-MAP partners targeting the integration of the BIG-MAP infrastructure in the European value chain for battery discovery and development.

Call conditions

The proposed projects should develop software tools, techniques, equipment or approaches that further strengthen the BIG-MAP infrastructure and must be made openly available to the battery community, e.g., in the BIG-MAP AppStore.

- **Topics:** The first round of proposals should be in one of the following areas:
 - 1) Develop APIs or interfaces between the BIG-MAP infrastructure and one of the LC-BAT-13/14/15-2020 projects
 - 2) Development of APIs/interfaces to software, techniques or equipment widely used in the battery community
 - 3) Development of apps for autonomous analysis of BIG-MAP data
 - 4) Apply the BIG-MAP infrastructure to further the develop of novel battery chemistries
- **Partners:** The project must include a minimum of 1 BIG-MAP partner and 1 external stakeholder.
- **Budget:** Expectedly around €50.000 for the BIG-MAP partner(s) and €50.000 for the external stakeholder(s). A maximum of 5 SI grants will be awarded in this round.
- **Duration:** 1-2 years, with an end date no later than July 1st, 2023.
- **Length:** 3 pages max plus the CV of the main PI from the BIG-MAP partner(s) and the main PI from the stakeholder(s).
- **Submission:** The proposals (max 20 Mb) must be submitted to BIG-MAP@dtu.dk by **Wednesday, April 7, 2021** to be eligible. Decisions of the allocation of funding are expected ultimo May, 2021.

Assessment procedure and criteria

The proposals will be evaluated by three independent experts and the Executive Board according to their:

- Value to BATTERY 2030+ and the European battery community
- Novelty and impact of the proposed idea or approach
- The competences of the PIs
- The feasibility of the project

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Conditions for the 1st SI applications



- Partners:
 - The project must include a **minimum of 1 BIG-MAP partner** and a **minimum of 1 external stakeholder**
- Budget:
 - Up to ~**€50.000** for the BIG-MAP partners and ~**€50.000** for the external stakeholder(s)
 - More partners can be included, but within a total budget of up to ~**€100.000**
 - An overview budget must be submitted (use [template](#))
 - Eligible costs: salary, running cost, equipment (detail budget for granted projects)
 - A maximum of 5 SI grants will be awarded in this round
- Project duration:
 - **1-2 years**, with an end date no later than **July 1st, 2023**
- Proposal length:
 - **3 pages** max plus the CV of the main PI from the BIG-MAP partner(s) and the main PI from the stakeholder(s)



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Conditions for the 1st SI proposals



- **Conditions:** The proposed projects should develop software tools, techniques, equipment or approaches that further strengthen the BIG-MAP infrastructure and should be made openly* available to the battery community, e.g., in the BIG-MAP App Store
 - Ex: an app adhering to the BattINFO ontology and the BIG-MAP data schema
- **Topics:** The first round of proposals should be in one of the following areas:
 - Develop APIs or interfaces between the BIG-MAP infrastructure and one of the LC-BAT-13/14/15-2020 projects
 - Development of APIs/interfaces to software, techniques or equipment widely used in the battery community
 - Development of apps for autonomous analysis of BIG-MAP data
 - Apply the BIG-MAP infrastructure to further the develop of novel battery chemistries



*) Open doesn't necessitate free. Externalizable, but could, e.g., be free to academics only

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Submission and Assessment



- **Submission:**

- The proposals (max. 20 Mb) must be submitted to BIG-MAP@dtu.dk by **Wednesday, April 7, 2021** to be eligible
- Decisions of the allocation of funding are expected ultimo May, 2021

- **Assessment procedure and criteria**

- The proposals will be evaluated by three independent experts and the BIG-MAP Executive Board according to their:
 - Value to BATTERY 2030+ and the European battery community
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What could an SI deliverable look like?



- A REST API like OPTIMADE (Casper Welzel Andreasen, EPFL)
- Working example of an Analysis App - Prisma (Eibar Flores, DTU)
- An Electronic Lab Notebook (CNRS, RS2E and collaborators)



DFT-VASP Quantum SimStack

Package name: dft-vasp
Current state: development (version 1.0)

The DFT-VASP WaNo implements a wide range of methods available within the VASP code.

[Show app details](#)



Format-Converter ASE SimStack

Package name: format-converter
Current state: development (version 1.0)

This app uses ASE technology to convert a geometry file from x to y format.

[Show app details](#)



OPTIMADE Web Client Materials Cloud Utilities

Package name: optimade-web
Current state: development

Graphical client hosted on Materials Cloud to search databases that implement the OPTIMADE API (<https://www.optimade.org/>).

[Show app details](#)



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BIG-MAP

PRISMA



Python-based, **R**obust, data-**I**ntensive **S**pectrum **M**onitoring **A**pp

Initial view



PRISMA: An app for the analysis of spectra

Load your time-dependent spectra, explore processing parameters within the user-friendly interface and apply your choices to process all spectra.

Your results are plot-ready: they are stored as .csv files recognized by all major scientific plotting software.

Eibar Flores, Technical University Denmark

▶ Choose a Pipeline

▶ Explore Processing Parameters

▶ Apply Parameters to all Spectra



Eibar Flores (DTU)



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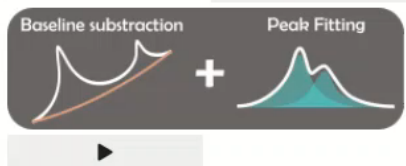


PRISMA: An app for the analysis of spectra

Eibar Flores, Technical University Denmark

BATTERY
20+30-

▼ Choose a Pipeline



▶ Explore Processing Parameters

▶ Apply Parameters to all Spectra



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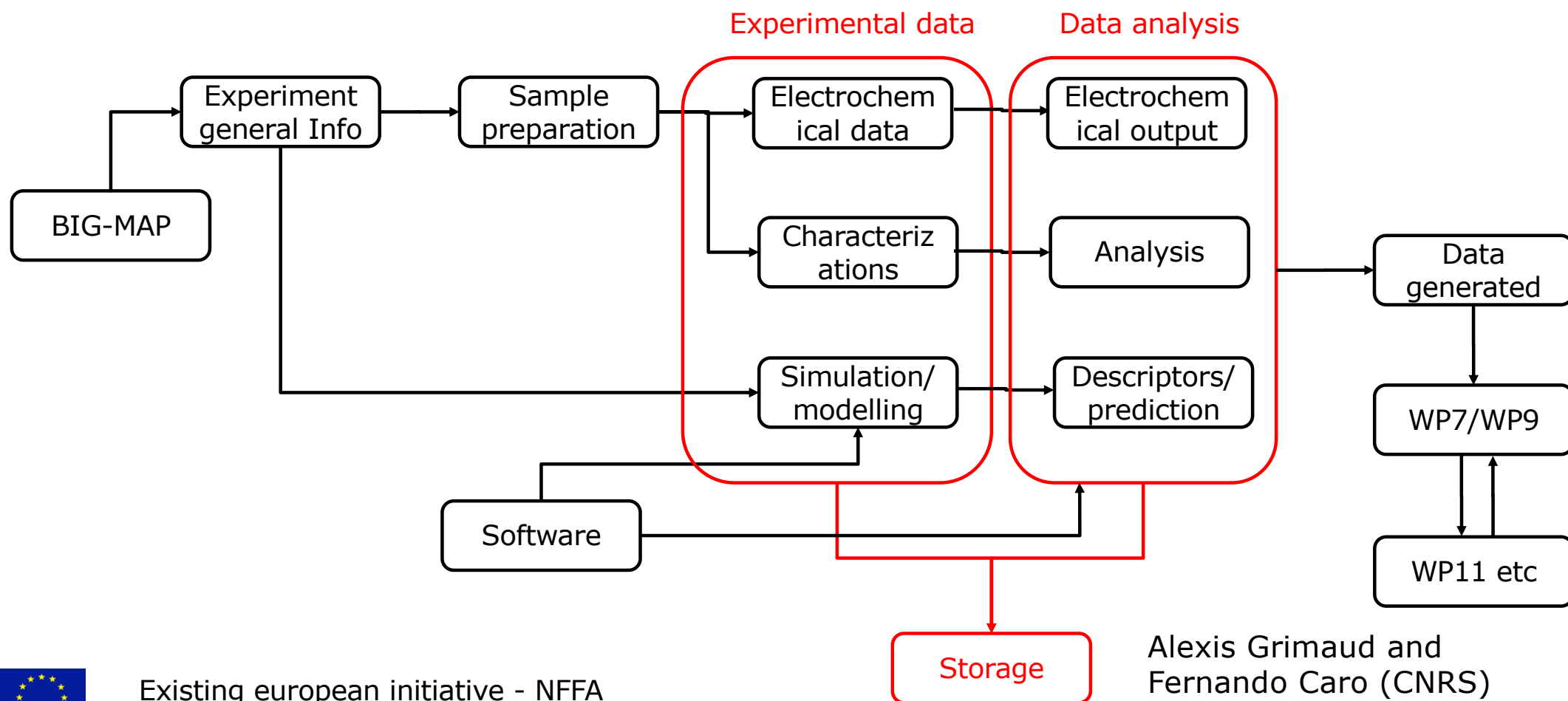
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Electronic Laboratory Notebook - Workflow



Existing european initiative - NFFA

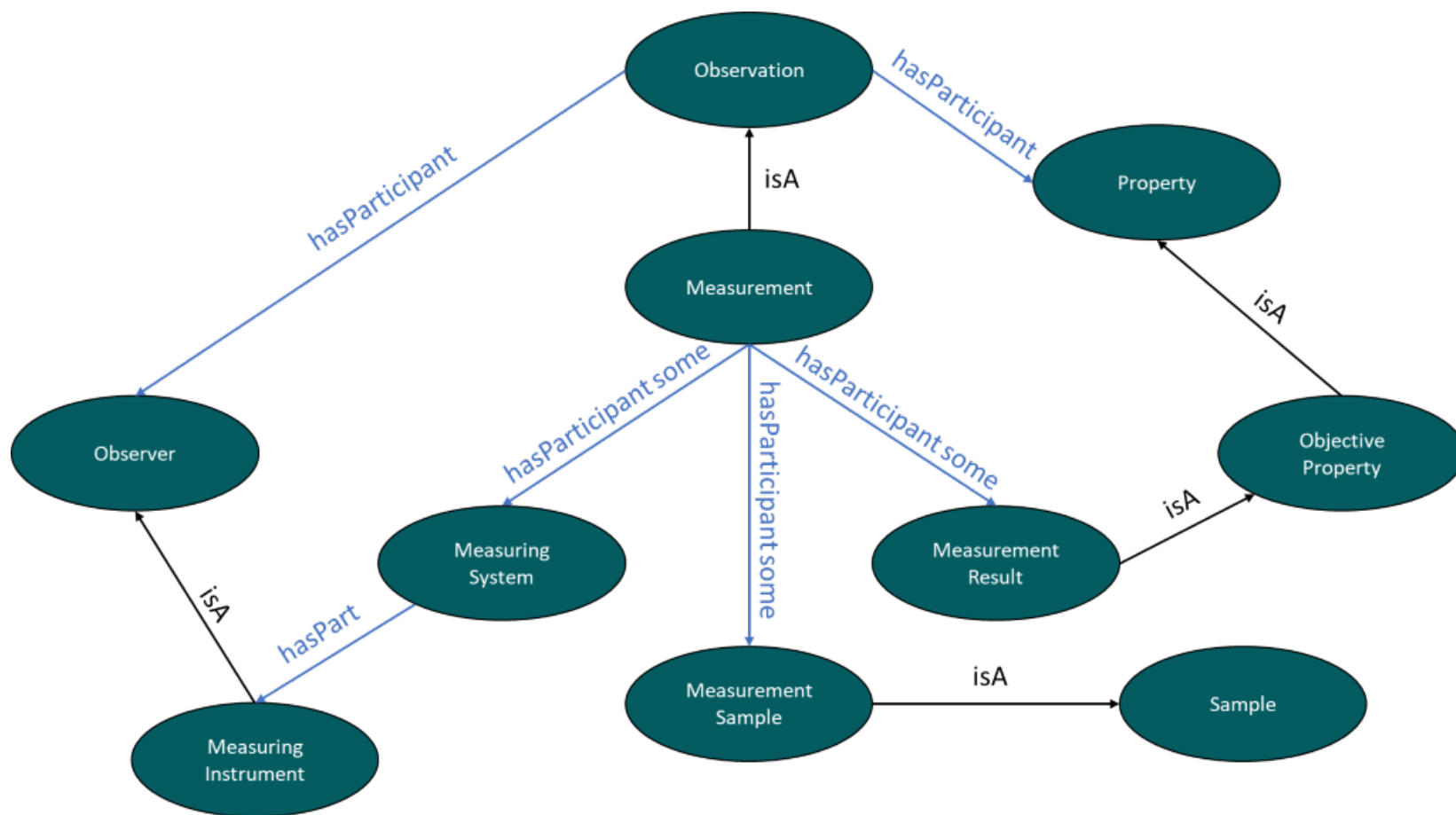
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Alexis Grimaud and
Fernando Caro (CNRS)

Eibar Flores (DTU)



Electronic Laboratory Notebook – using BattINFO



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Electronic Laboratory Notebook



Sample Technique **Data**

Raw Data

Describe the location and format of the raw data

Location Local PC Online

URL

Format of t...

Who to contact to access raw data: experimentalist or other

Experimentalist: raw data

Name

Email

Analysis Data

Describe the process, location, and format of the analyzed data

Location Local PC Online

URL

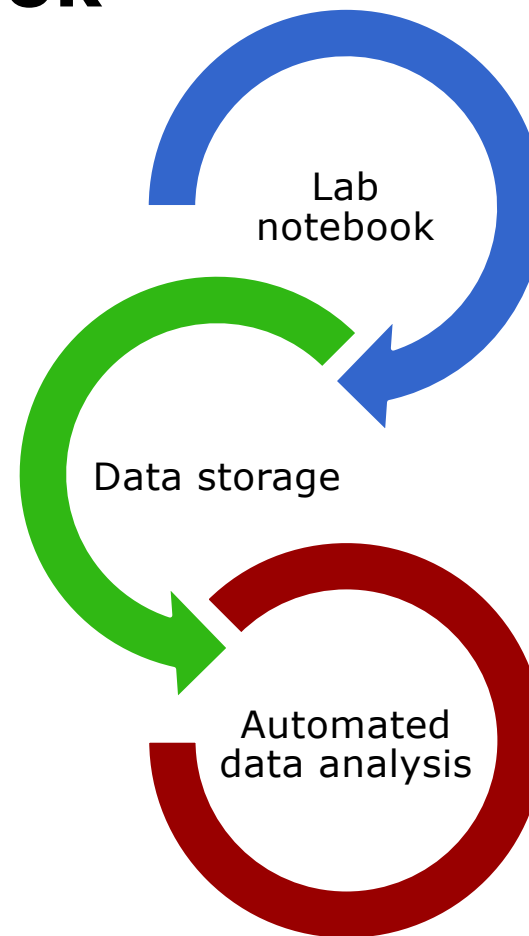
Format of t...

Who to contact to access analysis data: experimentalist or other

Experimentalist: analyzed data

Name

Email



Alexis Grimaud, Fernando Caro (CNRS)





How can you contribute?



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Q&A on the Stakeholder Initiatives



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BIG-MAP

BATTERY
20+30-

Wrap up



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Summary



- BIG-MAP: transitioning from sequential and Edisonian battery development to autonomous discovery of battery materials and interfaces/interphases
- AI-orchestrated acquisition of multi-fidelity data from simulations, machine learning and experiments to accelerate the discovery and synthesis process
- Establishing a common battery ontology (BattINFO), standards and protocols
- Develop externalizable tools for the European battery community (App Store)
- Creating closed-loop discovery workflows bridging simulations and experiments using uncertainty quantification
- Develop physics-aware spatio-temporal deep learning models for inverse design of battery materials and interfaces
- The Stakeholder Initiative call is now open for collaborative projects
- Special thanks to EMIRI and the BIG-MAP Management Support Team - and to you for joining our webinar!



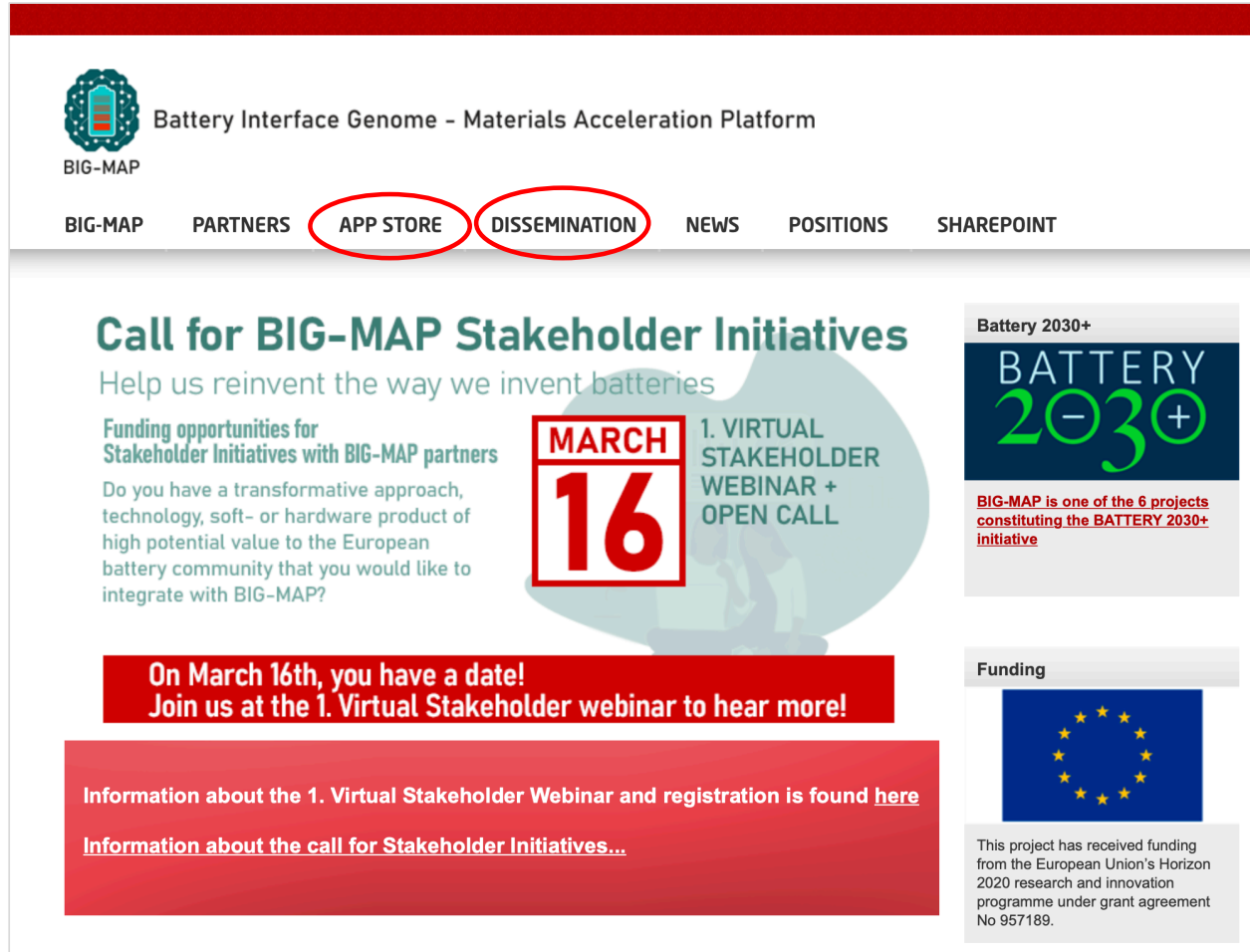
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Follow us on www.BIG-MAP.eu



The screenshot shows the website header with the BIG-MAP logo and navigation menu. The main content area features a call for stakeholder initiatives, a calendar for March 16th, and information about funding from the European Union. The navigation menu includes: BIG-MAP, PARTNERS, APP STORE, DISSEMINATION, NEWS, POSITIONS, and SHAREPOINT. The main content area has a red header bar. Below it, the BIG-MAP logo and name are followed by the text "Battery Interface Genome - Materials Acceleration Platform". The navigation menu is below that. The main content area features a large call for stakeholder initiatives, a calendar for March 16th, and information about funding from the European Union. The call for stakeholder initiatives includes the text "Call for BIG-MAP Stakeholder Initiatives" and "Help us reinvent the way we invent batteries". It also mentions "Funding opportunities for Stakeholder Initiatives with BIG-MAP partners" and "1. VIRTUAL STAKEHOLDER WEBINAR + OPEN CALL". The calendar shows "MARCH 16". The funding information includes the text "On March 16th, you have a date! Join us at the 1. Virtual Stakeholder webinar to hear more!" and "Information about the 1. Virtual Stakeholder Webinar and registration is found [here](#)". There are also two sidebars: "Battery 2030+" and "Funding". The "Battery 2030+" sidebar features the BATTERY 2030+ logo and the text "BIG-MAP is one of the 6 projects constituting the BATTERY 2030+ initiative". The "Funding" sidebar features the European Union flag and the text "This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189."



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...and on LinkedIn and Twitter: @BIGMAP_EU



The screenshot shows the LinkedIn profile page for 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'. The page header includes the LinkedIn logo, a search bar, and navigation icons for Home, My Network, Jobs, Messaging, Notifications, and Me. The profile name is 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)' with a 'Super admin view' button and a 'View as member' button. Below the name are tabs for 'All Pages', 'Content', 'Analytics', and 'Activity'. The main banner features the BIG-MAP logo, the text 'Battery 2030+ EU GA No. 957189', and 'Battery Interface Genome - Materials Acceleration Platform'. Below the banner is a description: 'A radical paradigm shift in battery innovation to lead a dramatic speed-up in battery discovery & innovation time.' and 'Research · Kongens Lyngby, Capital Region · 59 followers'. There are 'Edit Page' and 'Share Page' buttons. On the left, there is an 'Analytics' section showing '52 Unique visitors' and '0%'. In the center, there is a 'Start a post' section with options for Photo, Video, Document, and Poll. On the right, there is an 'Invite Connections To Follow' section showing '100/100 credits available' and a list of connections, with 'Christina' visible.

The screenshot shows the Twitter profile page for '@BIGMAP_EU'. The profile name is 'BIG-MAP' with 61 tweets. The bio states: 'BIG-MAP (Battery Interface Genome - Materials Acceleration Platform) is part of @2030Battery and funded by @EU_H2020 under grant No. 957189.' The location is 'Copenhagen, Denmark', the website is 'big-map.eu', and it was joined in 'June 2020'. There are 81 following and 445 followers. A list of followed accounts includes 'BASE - Batteries Sweden, Swiss Battery Days 2020/21, and 83 others you follow'. The page has tabs for 'Tweets', 'Tweets & replies', 'Media', and 'Likes'. A 'Pinned Tweet' is visible at the bottom.



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