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OPINCHARGE

Deliverable D6.2

Database

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29/05/2026	V1.1	Lukas Köbbing (DLR), Santhana Eswara (LIST), Beñat Larrarte-Lizarralde (CIDETEC)	Reviewed by DLR and LIST and small improvements were included by CIDETEC

Dissemination Level and Nature of the Deliverable		
SEN	Sensitive	PU - Public
Nature	R = Report, E = Ethics or, O = Other	DATA – data set, microdata, etc.

OPINCHARGE Consortium			
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1 Deliverable D6.2 Overview

Deliverable Name:

"**Database**"

2 Details on the performed work

The main objective of Task 6.2 and this deliverable is to establish a database framework that enables sharing proprietary data among project partners and facilitates its extension to the wider community. This is achieved by aligning with BATTERY2030+ and using the BIG-MAP Archive, as described in Section 2.1. Section 2.2 presents the open-access publications uploaded to the Zenodo platform.

In addition, a publicly accessible website has been developed to provide access to the Electrochemical Impedance Spectroscopy (EIS) methodology created in WP5 and detailed in D5.1, as described in Section 2.3.

2.1 FAIR criteria Database

The BIG-MAP Archive was established as a FAIR-compliant database to enable partners to share data within the project and the BATTERY2030+ community. Although the initial plan was to develop a dedicated framework exclusively for OPINCHARGE, this approach was revised during the early months of the project after participating in the "BIG-MAP Workshop towards a unified future," where the benefits of a unified framework were emphasized.

As a result, an OPINCHARGE group was created within the BIG-MAP Archive to facilitate data sharing among project partners. In addition, a new version of the framework introduced the option to assign licenses to shared data. These two changes made the framework suitable for the project's needs.

Table 1 summarizes all uploaded records.

Title	Authors	Date	License	Openness level	Total files	Total MB	Views	Downloads
Supporting data for "Slow Voltage Relaxation of Silicon Nanoparticles with a Chemo-Mechanical Core–Shell Model" (doi: 10.1021/acsami.4c12976)	Lukas Köbbing, Yannick Kuhn and Birger Horstmann	27/11/2024	BATTERY2030+ License	BATTERY2030	10	97.3	13	1
Supporting data for "Electrochemical Removal of HF from Carbonate-based LiPF6-containing Li-ion Battery Electrolytes (DOI: https://doi.org/10.1149/1945-7111/ad30d3)"	Xiaokun Ge, Marten Huck, Andreas Kuhlmann, Michael Tiemann, Christian Weinberger, Xiaodan	07/08/2024	BATTERY2030+ License	OPINCHARGE	21	220.1	8	0

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	Xu, Zhenyu Zhao and Hans-Georg Steinrünk							
Silicon Nanowires as Anodes for Lithium-Ion Batteries: Full Cell Modeling	Franziska Kilchert, Max Schammer, Arnulf Latz and Birger Horstmann	31/07/2024	BATTERY2030+ License	BATTERY2030	12	10.7	14	0
Task 1.4_Benchmarking_LFP cathode	Olatz Leonet and Álvaro Doñoro	21/07/2024	BATTERY2030+ License	OPINCHARGE	1	0.631	9	5

Table 1 Overview of all datasets uploaded to the BIG-MAP Archive and their key characteristics

2.2 Open access publications

Following the FAIR (Findable, Accessible, Interoperable, and Reusable) data principles defined within Task 6.2, all scientific publications generated during the project have been uploaded to the Zenodo platform. This ensures open accessibility, long-term preservation, and improved interoperability of the project results within the battery research community and BATTERY2030+ initiatives.

Table 2 summarises the publications currently available in the Zenodo repository:

Title	**Authors**	**Published Date**	**Views**	**Downloads**
Progress and perspectives on reference electrodes for Li-ion batteries	Álvaro Doñoro, Olatz Leonet, Ana Fernández-Barquín, Amaia Narbarte-Álvarez, Aroa R. Minar, Elixabete Ayerbe, Dennis Kopljar, Hans-Jürgen Grande, Idoia Urdampilleta and J. Alberto Blázquez	03/05/2026	2	5
Solid-State NMR Investigation of Electrolyte Effects on Silicon–Graphite Composite Anode: Solid Electrolyte Interphase Formation and Failure Mechanisms	Nahom Enkubahri Asres, Marta Cabello, Muhammad Khurram Tufail, Kerman Gomez Castresana, Aitor Villaverde and Juan Miguel López del Amo	23/04/2026	11	14
"X-ray Coulomb Counting" to Understand Electrochemical Systems	Chuntian Cao and Hans-Georg Steinrück	25/03/2026	2	2
X-ray reflectivity from micrometre-scaled surfaces using nanobeams	Vedran Vonk, Steffen Tober, Steven J. Leake, Breno Rabelo Coutinho Saraiva, Lisa Randolph, Arti Dangwal Pandey,	15/09/2025	3	4

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	Thomas F. Keller, Hans-Georg Steinrück and Andreas Stierle			
Operando visualization of Li distribution in solid-state batteries using focused ion beam-secondary ion mass spectrometry imaging	Sayantan Sharma, Alexander Santiago, Maria Martinez-Ibañez, Mathieu Gerard, Athira Suresh Kumar, Olivier De Castro, Tom Wirtz and Santhana Eswara	25/06/2025	79	58
Electrochemical Removal of HF from Carbonate-based LiPF6-containing Li-ion Battery Electrolytes*	Xiaokun Ge, Marten Huck, Andreas Kuhlmann, Michael Tiemann, Christian Weinberger, Xiaodan Xu, Zhenyu Zhao and Hans-Georg Steinrück	05/03/2025	146	144
Elliptical Silicon Nanowire Covered by the SEI in a 2D Chemo-Mechanical Simulation	Raphael Schoof, Lukas Köbbing, Arnulf Latz, Birger Horstmann and Willy Dörfler	24/01/2025	105	213
Dynamics of transition metal dissolution and cross-contamination in operating Lithium-ion batteries	Antonin Gajan, Kethsovann Var, Rajmohan Rajendiran, Jean-François Lemineur, Olivier Guiader, Benoit Mortemard de Boisse, Bernard Simon, Julien Demeaux and Ivan T. Lucas	17/12/2024	125	147
Slow Voltage Relaxation of Silicon Nanoparticles with a Chemo-Mechanical Core–Shell Model	Lukas Köbbing, Yannick Kuhn and Birger Horstmann	26/12/2024	139	181
Impact of Surface Enhanced Raman Spectroscopy in Catalysis	Andrei Stefancu, Javier Aizpurua, Ivano Alessandri, Ilko Bald, Jeremy J. Baumberg, Lucas V. Besteiro, Phillip Christopher, Miguel Correa-Duarte, Bart de Nijs, Angela Demetriadou, Renee R. Frontiera, Tomohiro Fukushima, Naomi J. Halas, Prashant K. Jain, Zee Hwan Kim, Dmitry Kurouski, Holger Lange, Jian-Feng Li, Luis M. Liz-Marzán, Ivan T. Lucas, Alfred J. Meixner, Kei Murakoshi, Peter Nordlander, William J. Peveler, Raul Quesada-Cabrera, Emilie Ringe, George C. Schatz, Sebastian Schlücker, Zachary D. Schultz, Emily Xi Tan, Zhong-Qun Tian, Lingzhi Wang, Bert M. Weckhuysen, Wei Xie, Xing Yi Ling, Jinlong Zhang, Zhigang Zhao, Ru-Yu Zhou and Emiliano Cortés	14/11/2024	121	113
Advanced methods for characterizing battery interfaces: Towards a comprehensive understanding of interfacial evolution in modern batteries	Israel Temprano, Javier Carrasco, Matthieu Bugnet, Ivan T. Lucas, Jigang Zhou, Robert S. Weatherup, Christopher A. O'Keefe, Zachary Ruff, Jiahui Xu,	13/09/2024 (uploaded:	4	5

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	Nicolas Folastre, Jian Wang, Antonin Gajan and Arnaud Demortière	30/04/2026)		
Investigation of Li accumulations in LLZO based solid state batteries via operando neutron imaging and ex-situ correlative structural and chemical analysis	Luca Cressa, Pierre Boillat, Mathieu Gerard, Yanyan Sun, Sayantan Sharma, Olivier De Castro, Maryam Nojabaee, Guido Schmitz, Tom Wirtz and Santhana Eswara	07/05/2024	113	100
Silicon Nanowires as Anodes for Lithium-Ion Batteries: Full Cell Modeling	Franziska Kilchert, Max Schammer, Arnulf Latz and Birger Horstmann	13/04/2024	124	227

*All data and complementary information are also shared

Table 2 Overview of all datasets uploaded to ZENODO and their key characteristics

2.3 Publicly accessible website for EIS analysis

This web application supports the analysis of Electrochemical Impedance Spectroscopy (EIS) data using Equivalent Circuit Modelling (ECM), Distribution of Relaxation Times (DRT), and Machine Learning (ML), and is based on a standard web architecture comprising backend, database, and frontend components. Figure 1 shows the overall web architecture.

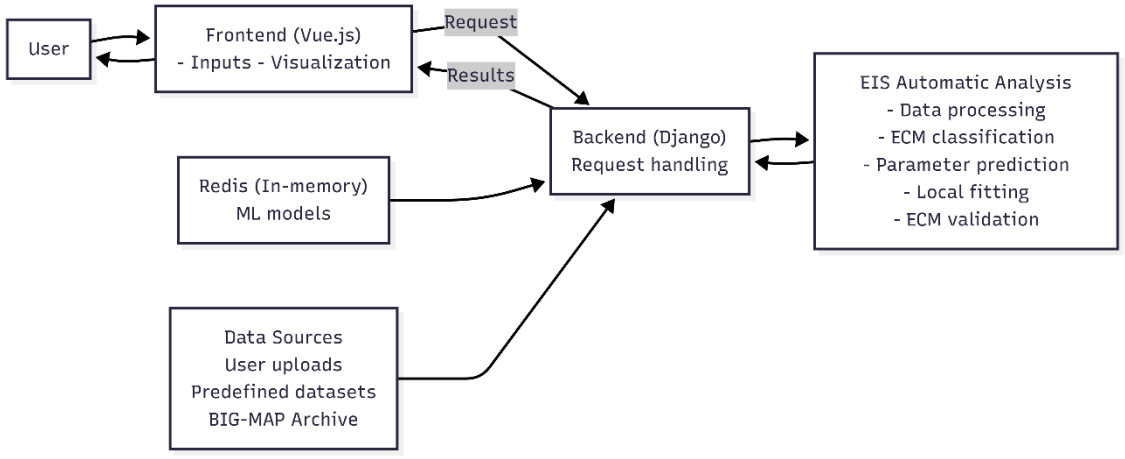

Figure 1 Overview of the web application workflow. The user uploads or selects raw data via the frontend, which sends requests to the backend. The backend performs EIS analysis using preloaded ML models from Redis, then returns results to the frontend for visualization. External datasets are accessed by the backend as needed.

The application was designed to balance performance and usability. Data-driven models are initialized in a Python environment at deployment and executed in memory during operation, avoiding repeated loading and reducing response time, at the cost of longer deployment. Redis is used to manage these preloaded models.

The frontend is intentionally authentication-free, allowing unrestricted access and simplifying user interaction, although preventing data persistence and personalization. As a result, user-defined configurations (e.g., custom ECMs) are session-based and not retained.

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Methodology. Development relied on GitHub for version control and Docker for deployment. The application is hosted on a local Ubuntu server at CIDETEC, with containerization ensuring reproducibility and isolation.

Backend. Built with Django, the backend integrates Task 5.2 models, handling requests, executing analyses, and returning structured results. Original EIS/DRT workflows were adapted from visual to structured outputs with minimal code changes. Parallel processing is enabled through multiple workers. Core functions include: (i) EIS/DRT analysis from multiple data sources (including BIG-MAP Archive), (ii) ECM classification via ML, (iii) parameter prediction and fitting, and (iv) validation of user-defined ECMs.

Database. No persistent storage is used; analyses are performed on demand. Redis serves only as an in-memory store for models.

Frontend. Developed with Vue.js, the interface enables data selection, configuration, and visualization of results (tables and interactive Nyquist, DRT, and Bode plots). It includes pages for general information, datasets, ECM descriptions, and the main analysis workflow, where users can also define and evaluate custom ECMs.

3 Summary

This report presents the development of a data-sharing and analysis framework within the project. The M12 milestone on a decentralized and interoperable database was achieved by aligning with BATTERY2030+ and adopting the BIG-MAP Archive, enabling FAIR-compliant data sharing among partners and extension to the wider community.

In parallel, a web application was developed to provide open access to advanced EIS analysis methodologies based on ECM, DRT, and machine learning. The platform, built with Django and Vue.js, runs preloaded models in memory using Redis for efficient performance. It is deployed via Docker, requires no user authentication, and performs on-demand analyses without persistent data storage.

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