A Linked Data Primer

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This project has received funding from the European Union's Horizon 2020 research and innovation initiative under grants agreement No 957189 (BIG-MAP) and No 957213 (BATTERY 2030+).



What are we trying to solve with linked data

How to link data

What can we do with linked data





Interaction between human actors

- Terminology
- Languages
- Requirements
- Technical background



Exchange of data

- Formats
- Metadata
- Methodology
- Postprocessing
- Access



Reproducibility

- Scope
- Inputs
- Methodology
- Pre-/post-processing
- Comparison
- Provenance



Interaction with autonomous machines

- Data Exchange format
- Metadata
- Safety and security
- Robustness



Linked data breaks barriers down by ensuring

- Enough context to understand data
- Enough information to reproduce results
- Streamlined interactions with hardware
- Streamlined exchange and access



How to link data

In 3 easy steps



Unique identifier: Sequence of characters uniquely identifying a resource used in the web. IDs must resolve to a document offering further data about the resource.





FINALES (09/2023) – Electrolyte Optimization for Maximum Conductivity and for Maximum Cycle Life

Bhowmik, Arghya¹; Busk, Jonas¹; Carlsson, Johan M.²; Castelli, Ivano E.¹; Clark, Simon³; Flores, Elbar³; Flowers, Jackson^{4,5}; Fuchs, Stefan^{4,6}; Gabetšček, Miran⁶; Hajiyani, Hamidreza²; Hanke, Felix⁷; Liot, François⁸; Merker, Leon^{4,5}; Pizzi, Giovanni^{8,9}; Ramirez, Francisco Fernando³; Riger, Laura Hannemose¹; Sain, Aeksed^{4,5}; Steensen, Simon¹; Stein, Helge S.^{4,5}; Vegge, Tejs¹; Vogler, Monika^{4,5}; Wölke, Christian¹⁰; Zhang, Bojing^{4,5}

Show affiliations

Description

This study investigates an electrolyte system composed of lithium hexafluorophosphate (LiPF6), ethylene carbonate (EC) and ethyl methyl carbonate (EMC). For the assembly of full cells, electrodes based on graphite and lithium nickel dioxide (LNO) are used. This work provides insight into the similarity of formulations of an electrolyte optimized for maximum conductivity and another one optimized for maximum cycle life are expected to be in this chemical system. The goal is to assess whether it is promising to target research efforts on finding an electrolyte formulation within this chemical space which can full both requirements.





Concept 🖻 Open Access 🛛 🐵 🕥

Data Management Plans: the Importance of Data Management in the BIG-MAP Project**

Prof. Ivano E. Castelli 🕵 Dr. Daniel J. Arismendi-Arrieta. Prof. Arghya Bhowmik, Dr. Isidora Cekic-Laskovic. Dr. Simon Clark, Prof. Robert Dominko, Dr. Eibar Flores, Jackson Flowers ... See all authors 🗸

First published: 28 August 2021 | https://doi.org/10.1002/batt.202100117 | Citations: 14

*** BIG-MAP: Battery Interface Genome – Materials Acceleration Platform. A previous version of this manuscript has been deposited on a preprint server (DOI: http://arxiv.org/abs/2106.01616)

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Graphical Abstract

FAIR play: Standardization and ontology have the role of homogenizing the data and make them interoperable. Data Management Plans are increasingly important for accelerating research. Here, we describe the second seco



Controlled vocabulary: List of concepts of predefined, agreed and curated terms with unambiguous meaning. Concepts themselves must be uniquely identified (URLs).



Web vocabularies: digital resources Datasets, file formats, images, multimedia, events, locations, persons, software, ...



BattINFO: batteries + electrochemistry Voltage, current, EIS, CCCV, Battery, Electrode, Active Material, LFP, NCM, SEI, Lithium Plating ...



BattINFO: a machine-readable description of concepts in batteries and electrochemistry.



Concepts are organized as a network: Nodes: Battery Concepts Edges: relations among concepts

Provides:

- The vocabulary to index battery data
- The connections representing battery knowledge



Schema.org: a machine-readable description of web resources



Concepts are organized as hierarchy: Nodes: Web Concepts Edges: Relations among concepts

Provides:

- The vocabulary to describe and index web resources
- Interoperability for search engines (e.g. google)



Additional vocabularies: tailored to some domains.

CSVW Namespace Vocabulary Terms W3C Document 06 June 2017



Describes: CSV (tabular) files Maintainer: W3C Prefix: "csvw"

CHAMEO

Describes: Characterization of materials **Maintainer:** EMMC Task Force **Prefix:** "chameo"

DublinCore

Describes: Web resources Maintainer: The Dublin Core[™] Metadata Initiative Prefix: "dc" EUropean Research Information Ontology (EURIO)



Describes: Research projects Maintainer: European Union Vocabularies Prefix: "eurio"



JSON-LD: Method of annotating and linking data with the widely-used, machine-readable JSON format.

Test.csv

Col 1	Col 2	Col 3

Test_metadata.jsonld

Annotations become entries in the hierarchy of JSON fields

Annotations might live:

- Within the same data file (e.g. HDF5)
- As a separate accompanying file to the data
- All data, metadata and annotations in single JSON file



Do I have to write all these annotations manually?

Hopefully NOT: we build User Interfaces to make annotations user-friendly



Test_metadata.jsonld

"@context": "https://mydomain.com/context.json" "csvw:tableSchema": { "csvw:columns": ["csvw:name": "time", "csvw:titles": "Time / s", "csvw:propertyUrl": { "@type": "Time",...},...} "csvw:name": "voltage", "csvw:titles": "Voltage / V", "csvw:propertyUrl": { "@type": "CellVoltage" },



Linked data: what can we do with it?





What can we do with Linked Data Make network accessible in Knowledgebase



URI: https://institution.com/api/battexp









Linked data

- 1. Uniquely identified and referencing other data (URLs)
- 2. Annotated with controlled vocabularies (Ontologies)
- In a machine-readable format supporting annotations (JSON-LD)

Linked data enables reproducing, exchanging and automating battery research.



Technology for a better society