

Towards an autonomous robotic battery materials research platform powered by automated workflow and ontologized FAIR data management

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Vision towards autonomous battery research





Aurora battery assembly and cycling robot



Developed in collaboration with 🧧



Automated coin cell assembly robot

- Assembly of 32 coin cells per batch
- Automated electrode balancing
- Mixing of 32 electrolyte formulations

Automated coin cell cycling

- 256 dedicated potentiostat channels
- Real-time control of cell cycling parameters
- On-the-fly monitoring of cell cycling data



Proof-of-concept 10 generations à 32 cells



- Validation with NMC622 vs graphite cells in 1M LiPF₆ in EC:EMC 3:7
- Formation cycling at C/10, long-term cycling at 1C
- 32 cells split into groups of 8 cells cycled to different upper cut-off voltage

Kraus et al. J. Mater. Chem. A, 2024, 12, 10773 https://dgbowl.github.io/



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Automated workflow



Automated Battery Cycling: Tomato manages and monitors battery cycling Integrated Workflow: Ensures seamless data flow from design to analysis Real-time Monitoring: Maintains experiment accuracy and consistency Graphical user interface: Easy to use

Kraus et al. J. Mater. Chem. A, 2024, 12, 10773 https://dgbowl.github.io/ https://big-map.github.io/big-map-registry/apps/aiidalab-aurora.html



Aiida lab user interface

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- Visualize metadata for each battery cell in a generation
- Specify cycling protocol for individual cells or groups of cells
- Batch submission and monitoring of cells during cycling

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Aiida lab user interface



- Retrieve and analyze battery cycling data
- Assess and compare performance of single cells and multiple cells
- Various plot types including swarm plots

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Why ontologized FAIR data?



- (Meta)data are assigned a globally unique and persistent identifier
- (Meta)data are retrievable by their identifier via open, free protocols
- (Meta)data meet domain-relevant community standard



Ontologizing your own battery data

Non-ontologized metadata

Data description	Data value	Date unit
Cathode gravimetric discharge capacity	167	mAh/g

Ontologized metadata



- BattINFO ontology provides shared vocabulary and taxonomy
- BattINFO defines the properties, attributes, and relationships of battery-related concepts
- BattINFO ontology enables semantic searches

https://githbub.com/BIG-MAP/BattINFO S. Clark et al. Adv. Energy Materials 2022, 2102702



Ontologizing your own battery data

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BattINFO Converter

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- Convert tabulated (meta)data in Excel format into JSON-LD, simply by drag and drop!
- Excel (meta)data schema template for standard coin cell ready for download
- Additional (meta)data schema templates (e.g. solid-state batteries) in development

https://battinfoconverter.streamlit.app/

Plainpan et al. in preparation



BattINFO Coin Cell Battery Schema

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- Excel (meta)data schema easy to fill if you know how to build a coin cell
- ~30 required, ~15 recommanded, ~100 optional metadata items
- Pre-filled example for a NMC622/graphite cell with 1M LiPF6 in EC:EMC 3:7 by vol



BattINFO Coin Cell Battery Schema

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- Can be adapted easily respecting the BattINFO ontology
- Can be pre-filled with your default configuration values
- Lock certain fields to avoid unintentional errors

https://battinfoconverter.streamlit.app/

Conclusions

- Aurora robotic platform for battery research equipped with automated coin cell assembly, electrode balancing, electrolyte mixing, and battery cell cycling with 256 channels.
- Aiida workflow manager offering full data provenance and graphical user interface.
- BattINFO Converter ontologizes your own battery data



European

Batteries





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PREMISE