

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

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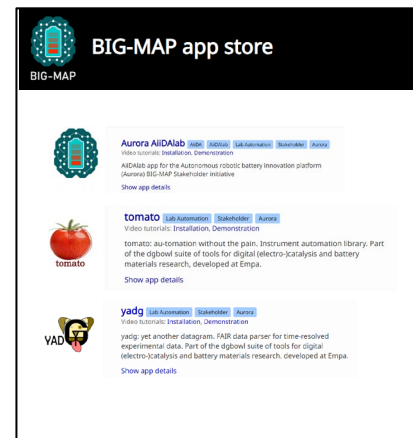
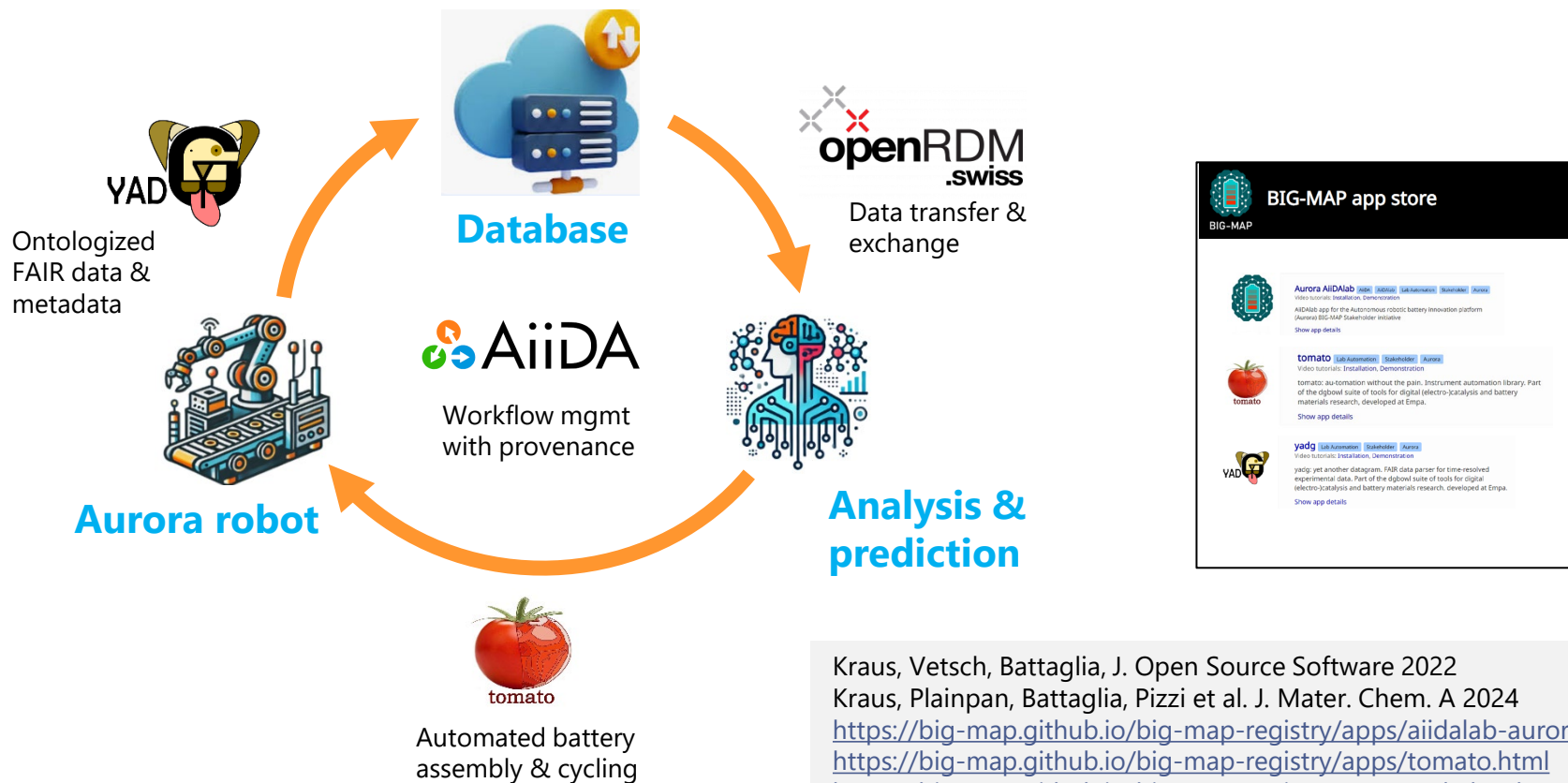
³ EPFL, School of Engineering, Institute of Materials

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⁵ now at Technische Universität Berlin

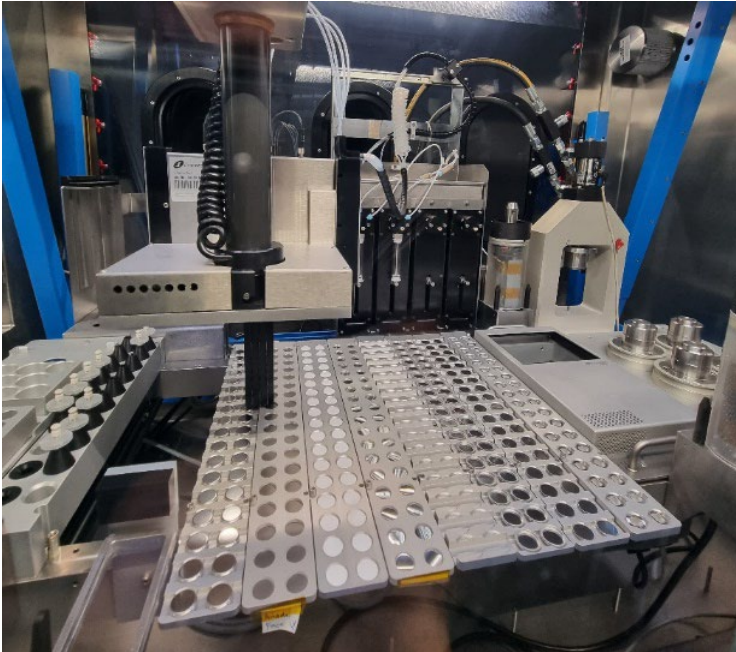


Vision towards autonomous battery research



Kraus, Vetsch, Battaglia, J. Open Source Software 2022
 Kraus, Plainpan, Battaglia, Pizzi et al. J. Mater. Chem. A 2024
<https://big-map.github.io/big-map-registry/apps/aiidalab-aurora.html>
<https://big-map.github.io/big-map-registry/apps/tomato.html>
<https://big-map.github.io/big-map-registry/apps/yadg.html>

Aurora battery assembly and cycling robot



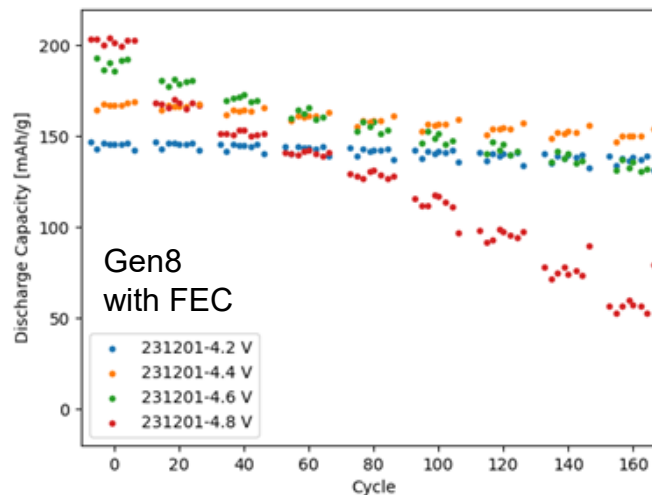
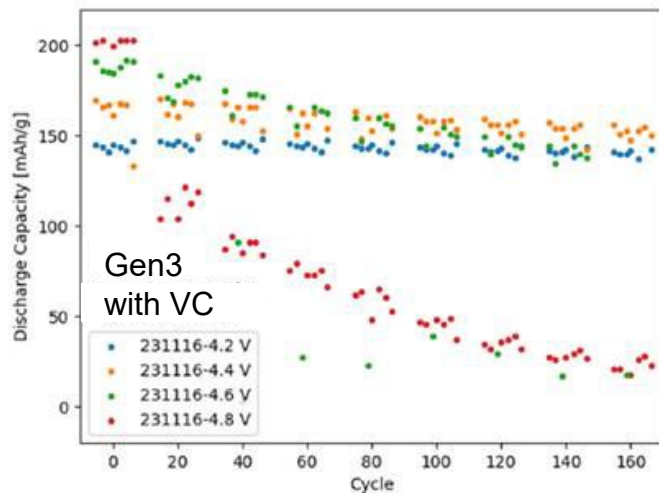
Automated coin cell assembly robot

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

Automated coin cell cycling

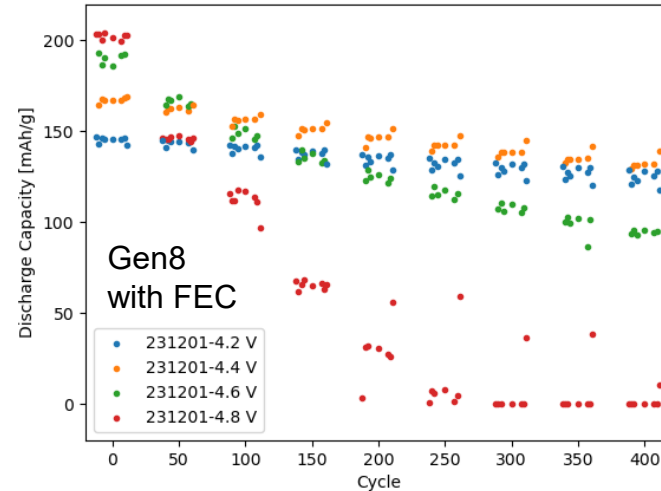
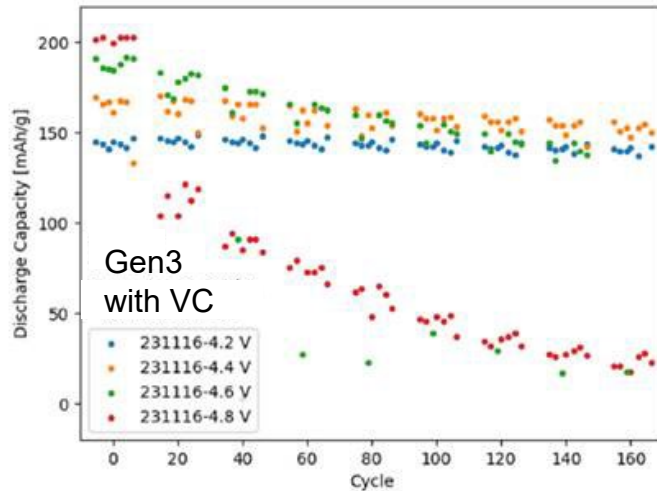
- 256 dedicated potentiostat channels
- Real-time control of cell cycling parameters
- On-the-fly monitoring of cell cycling data

Proof-of-concept 10 generations à 32 cells



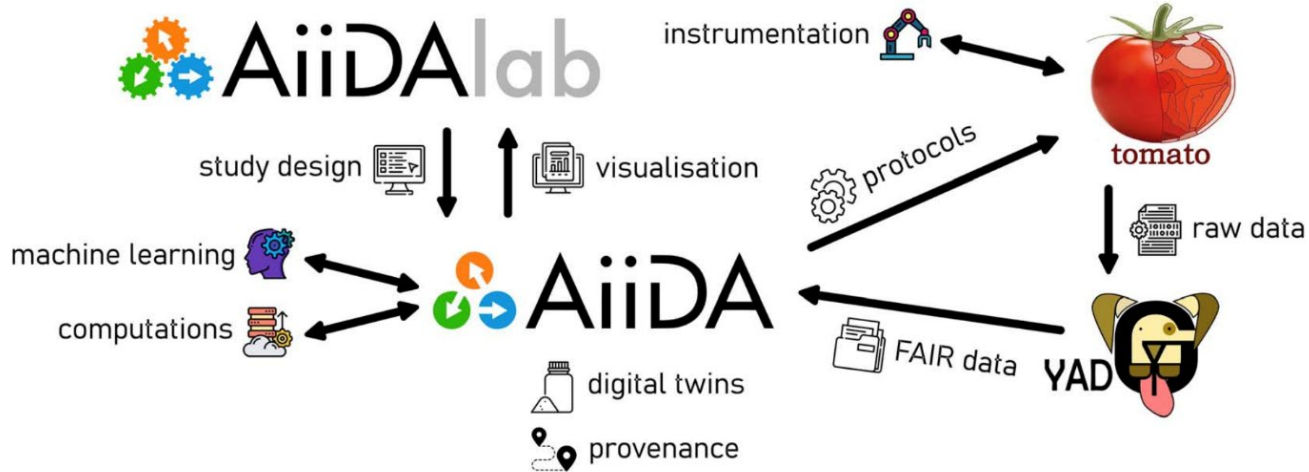
- Validation with NMC622 vs graphite cells in 1M LiPF₆ in EC:EMC 3:7
- Formation cycling at C/10, long-term cycling at 1C
- 32 cells split into groups of 8 cells cycled to different upper cut-off voltage

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

Automated workflow



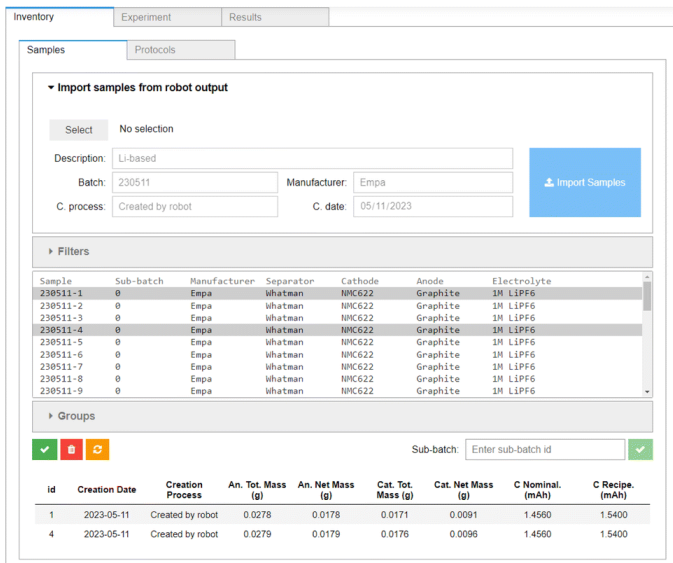
Automated Battery Cycling: Tomato manages and monitors battery cycling

Integrated Workflow: Ensures seamless data flow from design to analysis

Real-time Monitoring: Maintains experiment accuracy and consistency

Graphical user interface: Easy to use

Aiida lab user interface



Import samples from robot output

Select: No selection

Description: Li-based

Batch: 230511 Manufacturer: Empa

C. process: Created by robot C. date: 05/11/2023

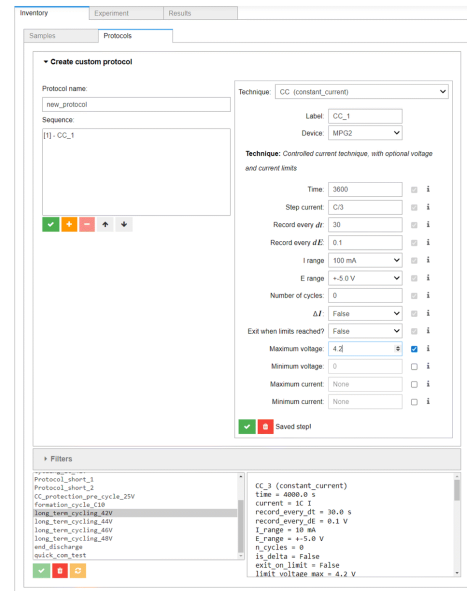
Filters

Sample	Sub-batch	Manufacturer	Separator	Cathode	Anode	Electrolyte
230511-1	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-2	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-3	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-4	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-5	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-6	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-7	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-8	0	Empa	Whatman	NKC622	Graphite	1M LiPF6
230511-9	0	Empa	Whatman	NKC622	Graphite	1M LiPF6

Groups

Sub-batch: Enter sub-batch id

Id	Creation Date	Creation Process	An. Tot. Mass (g)	An. Net Mass (g)	Cat. Tot. Mass (g)	Cat. Net Mass (g)	C Nominal. (mAh)	C Recipe. (mAh)
1	2023-05-11	Created by robot	0.0278	0.0178	0.0171	0.0091	1.4560	1.5400
4	2023-05-11	Created by robot	0.0279	0.0179	0.0176	0.0096	1.4560	1.5400



Create custom protocol

Protocol name: New protocol

Sequence: [1]-CC_1

Technique: CC (constant_current)

Label: CC_1

Device: MPQ2

Technique: Controlled current technique, with optional voltage and current limits

Time: 3600

Step current: C0

Record every dI: 30

Record every dE: 0.1

I range: 100 mA

E range: +/-5.0 V

Number of cycles: 0

ΔI: False

Exit when limits reached?: False

Maximum voltage: 4.2

Minimum voltage: 0

Maximum current: None

Minimum current: None

Filters

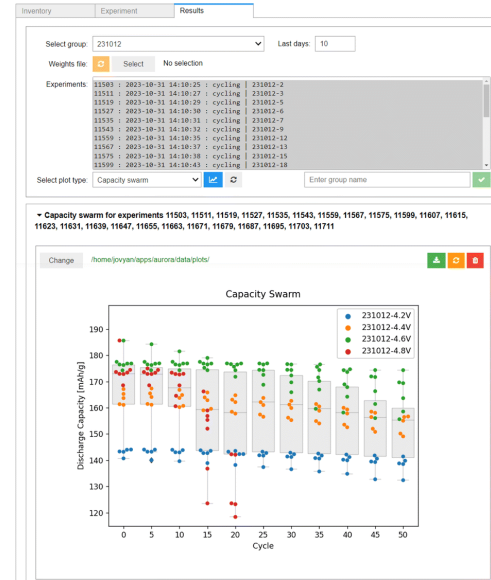
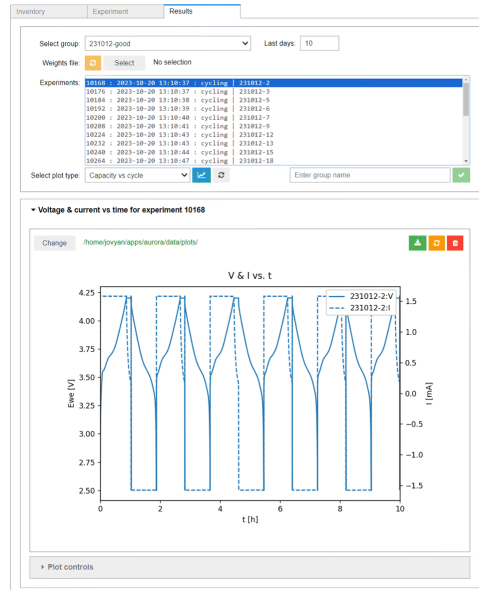
```

Protocol_short_1
Protocol_shor_1
CC_production_001_cy_25V
Formation_cy_1_18
long_term_cycling_48V
long_term_cycling_48V
long_term_cycling_48V
long_term_cycling_48V
end_of_charge
exit_on_test

CC_1 (constant current)
time = 4800.0 s
current = IC I
record_every_dI = 30.0 s
record_every_dE = 0.1 V
I_range = 10 mA
E_range = +/-5.0 V
n_cycles = 0
is_delta = false
exit_on_limit = false
limit_voltage_max = 4.2 V
  
```

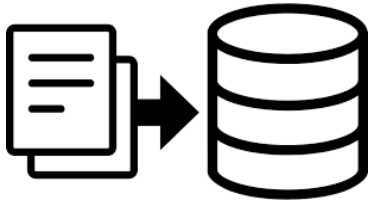
- Visualize metadata for each battery cell in a generation
- Specify cycling protocol for individual cells or groups of cells
- Batch submission and monitoring of cells during cycling

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

Why ontologized FAIR data?



Findability
Accessibility
Interoperability
Reusability

- (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

Ontologizing your own battery data

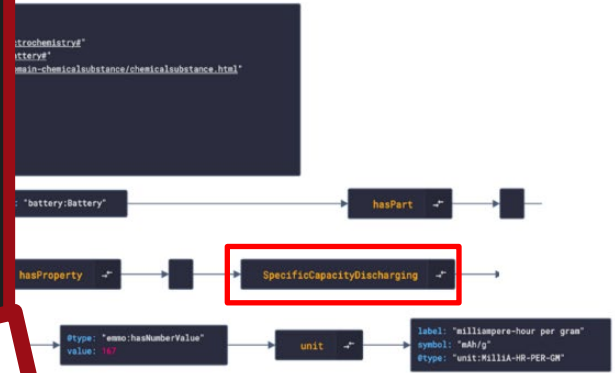
Non-ontologized metadata


Data description	Data value
Cathode gravimetric discharge capacity	167

```

1  {
2  "@context": {
3  "schema": "https://schema.org",
4  "emmo": "https://w3id.org/emmo#",
5  "echem": "https://w3id.org/emmo/domain/electrochemistry#",
6  "battery": "https://w3id.org/emmo/domain/battery#",
7  "chemical": "https://emmo-repo.github.io/domain-chemicalsubstance/chemicalsubstance.html",
8  "unit": "https://qudt.org/vocab/unit/",
9  "id": "For indexing purpose",
10 "hasPart": "emmo:hasPart",
11 "hasProperty": "emmo:hasProperty",
12 "hasQuantity": "emmo:hasQuantity",
13 "hasNumberValue": "emmo:hasNumberValue",
14 "hasComponent": "emmo:hasComponent"
15 },
16 "Battery": {
17 "@type": "battery:Battery",
18 "hasPart": {
19 "Cathode": {
20 "@type": "echem:Cathode",
21 "hasProperty": {
22 "SpecificCapacityDischarging": {
23 "@type": "echem:SpecificCapacityDischarging",
24 "hasNumberValue": {
25 "@type": "emmo:hasNumberValue",
26 "value": 167,
27 "unit": {
28 "label": "milliampere-hour per gram",
29 "symbol": "mAh/g",
30 "@type": "unit:Millia-HR-PER-G"
31 }
32 }
33 }
34 }

```



Manually ontologizing your data is laborious and prone to errors 

- BattINFO ontology is not comprehensive enough to cover all types of battery-related concepts
- BattINFO definition is not precise enough to support semantic searches

BattINFO Converter



BattINFO converter

App Version: 0.1.0

Upload your metadata Excel file here

Drag and drop file here
Limit 200MB per file • XLSX, XLSM

Browse files

Ontologizing your metadata can significantly enhance the interoperability of data across various research groups. To learn more about ontologizing your metadata, we invite you to visit our page on [metadata](#). While the benefits of this process are clear, it can often be a daunting task. In our mind, we've developed an BattINFO converter web application that simplifies this intricate task, making it more manageable.

BattINFO converter helps you ontologize metadata.

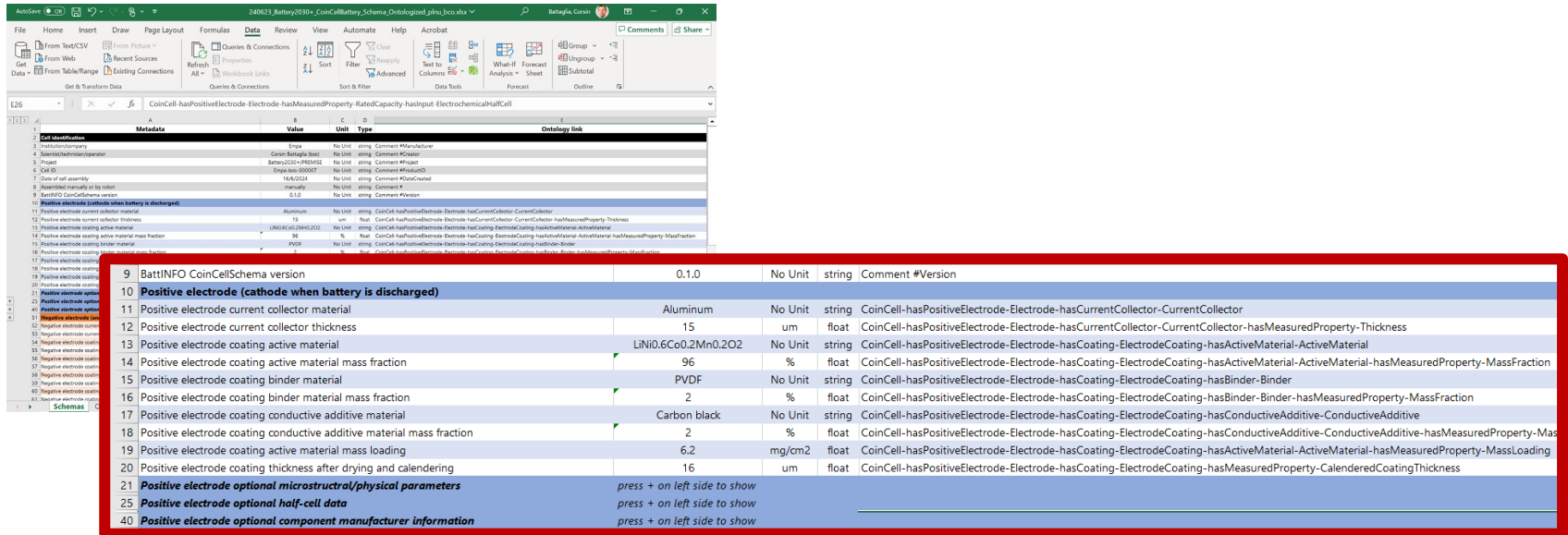
```

{
  "@context": {
    "schema": "https://schema.org",
    "emmo": "https://w3id.org/emmo",
    "echem": "https://w3id.org/emmo/domain/electrochemistry",
    "battery": "https://w3id.org/emmo/domain/battery",
    "chemical": "https://emmo-repo.github.io/domain-chemical-substance/chemical-substance.html",
    "unit": "https://qudt.org/vocab/unit/",
    "isac": "for indexing purpose",
    "hasPart": "emmo:hasPart",
    "hasProperty": "emmo:hasProperty",
    "hasQuantity": "emmo:hasQuantity",
    "hasNumberValue": "emmo:hasNumberValue",
    "hasComponent": "emmo:hasComponent"
  },
  "battery": {
    "@type": "battery:Battery",
    "Cathode": {
      "@type": "echem:Cathode",
      "hasProperty": {
        "SpecificCapacityDischarging": {
          "@type": "echem:SpecificCapacityDischarging",
          "hasNumberValue": {
            "@type": "emmo:hasNumberValue",
            "value": 167,
            "unit": {
              "@type": "milliampere-hour per gram",
              "unit": "mAh/g"
            }
          }
        }
      }
    }
  }
}

```

- 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

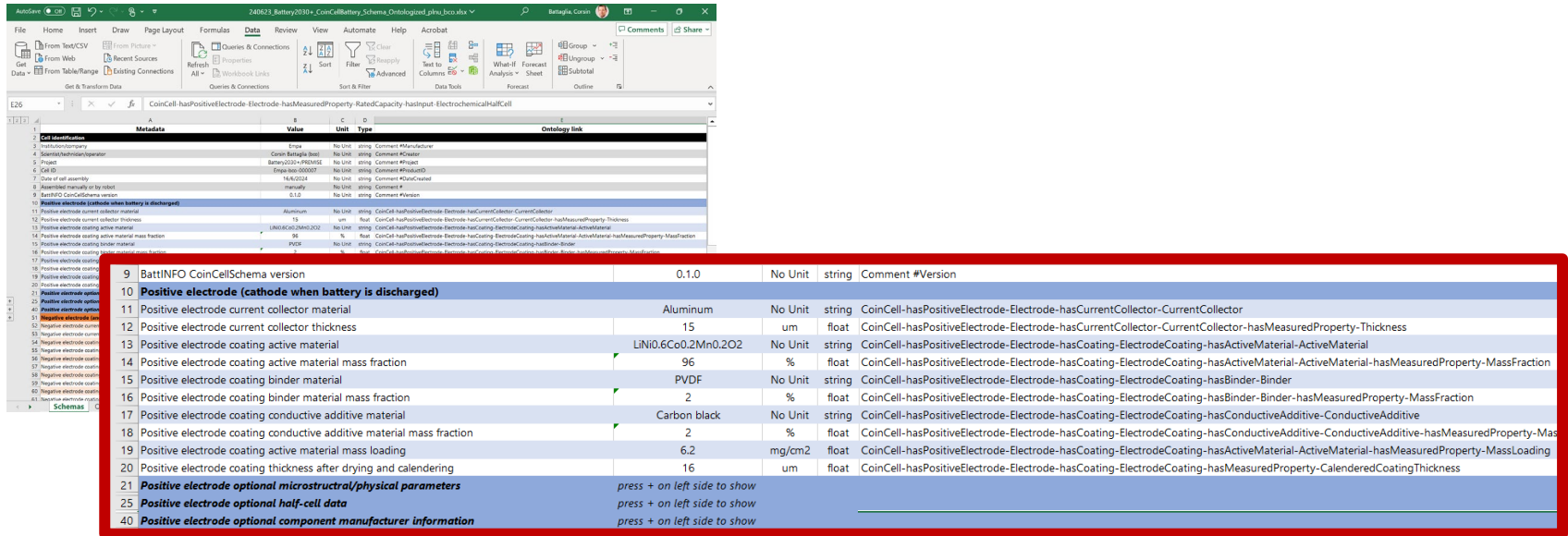
BattINFO Coin Cell Battery Schema



Metadata	Value	Unit	Type	Ontology link
9	BattINFO CoinCellSchema version	0.1.0	No Unit	string Comment #Version
10	Positive electrode (cathode when battery is discharged)			
11	Positive electrode current collector material	Aluminum	No Unit	string CoinCell-hasPositiveElectrode-Electrode-hasCurrentCollector-CurrentCollector
12	Positive electrode current collector thickness	15	um	float CoinCell-hasPositiveElectrode-Electrode-hasCurrentCollector-CurrentCollector-hasMeasuredProperty-Thickness
13	Positive electrode coating active material	LiNi0.6Co0.2Mn0.2O2	No Unit	string CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasActiveMaterial-ActiveMaterial
14	Positive electrode coating active material mass fraction	96	%	float CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasActiveMaterial-ActiveMaterial-hasMeasuredProperty-MassFraction
15	Positive electrode coating binder material	PVDF	No Unit	string CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasBinder-Binder
16	Positive electrode coating binder material mass fraction	2	%	float CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasBinder-Binder-hasMeasuredProperty-MassFraction
17	Positive electrode coating conductive additive material	Carbon black	No Unit	string CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasConductiveAdditive-ConductiveAdditive
18	Positive electrode coating conductive additive material mass fraction	2	%	float CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasConductiveAdditive-ConductiveAdditive-hasMeasuredProperty-MassFraction
19	Positive electrode coating active material mass loading	6.2	mg/cm2	float CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasActiveMaterial-ActiveMaterial-hasMeasuredProperty-MassLoading
20	Positive electrode coating thickness after drying and calendaring	16	um	float CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasMeasuredProperty-CalenderedCoatingThickness
21	Positive electrode optional microstructural/physical parameters			<i>press + on left side to show</i>
25	Positive electrode optional half-cell data			<i>press + on left side to show</i>
40	Positive electrode optional component manufacturer information			<i>press + on left side to show</i>

- Excel (meta)data schema easy to fill if you know how to build a coin cell
- ~30 required, ~15 recommended, ~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



Metadata	Value	Unit	Type	Ontology link	
9	BattINFO CoinCellSchema version	0.1.0	No Unit	string	Comment #Version
10	Positive electrode (cathode when battery is discharged)				
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12	Positive electrode current collector thickness	15	um	float	CoinCell-hasPositiveElectrode-Electrode-hasCurrentCollector-CurrentCollector-hasMeasuredProperty-Thickness
13	Positive electrode coating active material	LiNi0.6Co0.2Mn0.2O2	No Unit	string	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasActiveMaterial-ActiveMaterial
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15	Positive electrode coating binder material	PVDF	No Unit	string	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasBinder-Binder
16	Positive electrode coating binder material mass fraction	2	%	float	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasBinder-Binder-hasMeasuredProperty-MassFraction
17	Positive electrode coating conductive additive material	Carbon black	No Unit	string	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasConductiveAdditive-ConductiveAdditive
18	Positive electrode coating conductive additive material mass fraction	2	%	float	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasConductiveAdditive-ConductiveAdditive-hasMeasuredProperty-MassFraction
19	Positive electrode coating active material mass loading	6.2	mg/cm2	float	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasActiveMaterial-ActiveMaterial-hasMeasuredProperty-MassLoading
20	Positive electrode coating thickness after drying and calendaring	16	um	float	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasMeasuredProperty-CalenderedCoatingThickness
21	Positive electrode optional microstructural/physical parameters				<i>press + on left side to show</i>
25	Positive electrode optional half-cell data				<i>press + on left side to show</i>
40	Positive electrode optional component manufacturer information				<i>press + on left side to show</i>

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

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



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Edan Bainglass
Giovanni Pizzi
Nicola Marzari

Simon Clark
Eibar Flores

Amira Abou-Hamdan
And team



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