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

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BIG-MAP BATTERY 2030+ PREMISE ETH BOARD

Vision towards autonomous battery research

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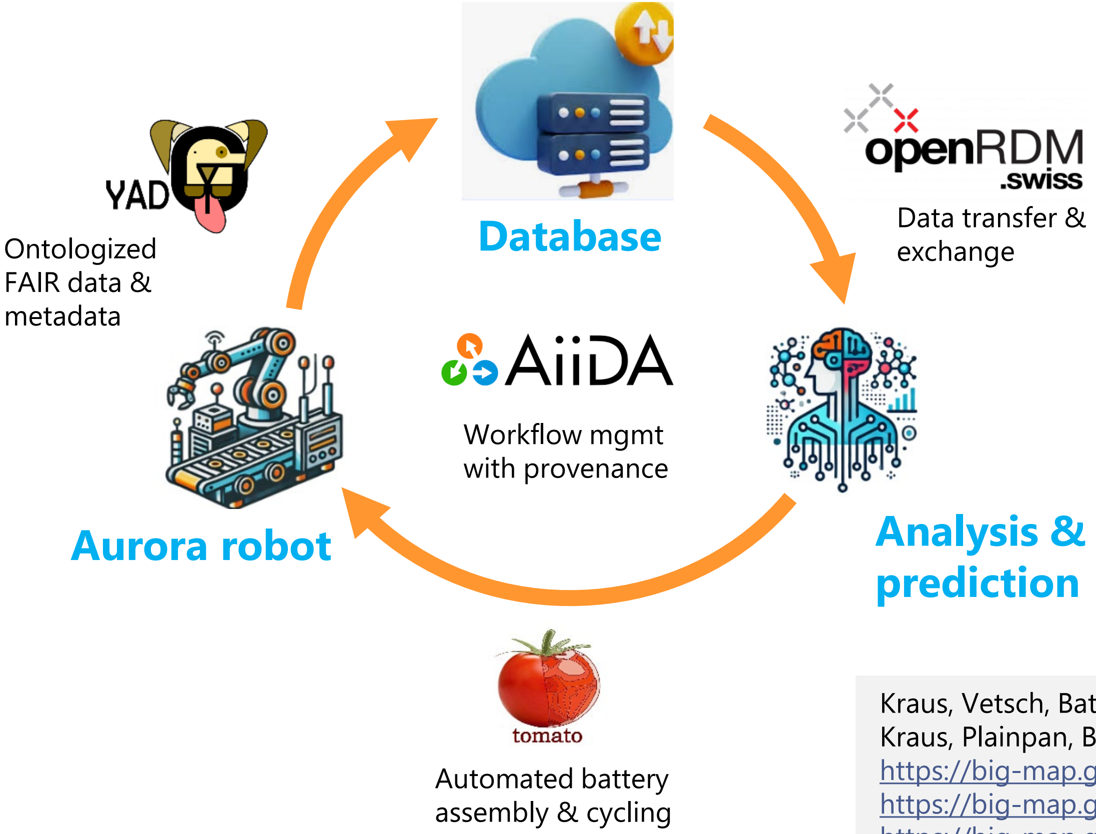

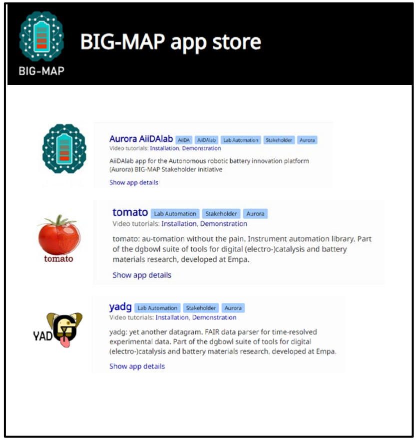

Kraus, Vetsch, Battaglia, J. Open Source Software 2022
Kraus, Plainpan, Battaglia, Pizzi et al. J. Mater. Chem. A 2024
https://big-map.github.io/big-map-registry/apps/aiidalab-aurora.html
https://big-map.github.io/big-map-registry/apps/tomato.html
https://big-map.github.io/big-map-registry/apps/yadg.html

Aurora battery assembly and cycling robot

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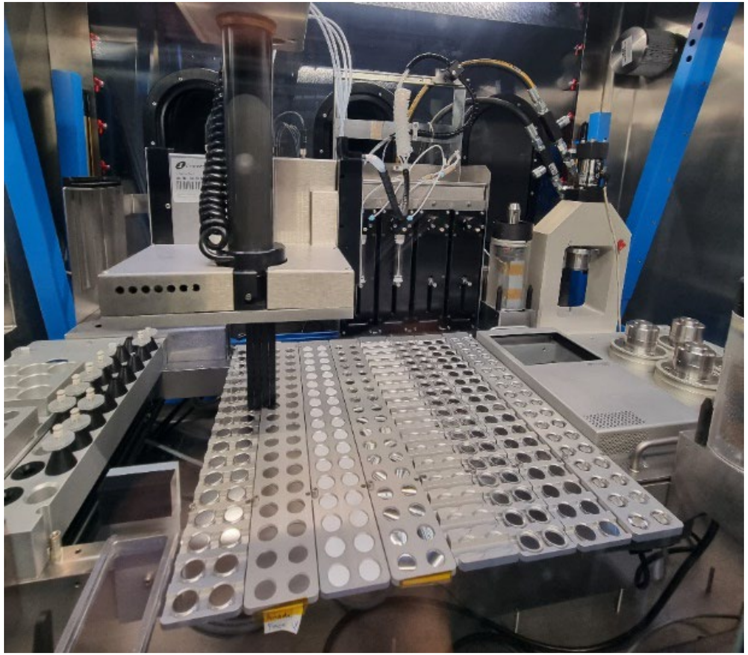


Developed in collaboration with CHEMSPEED TECHNOLOGIES

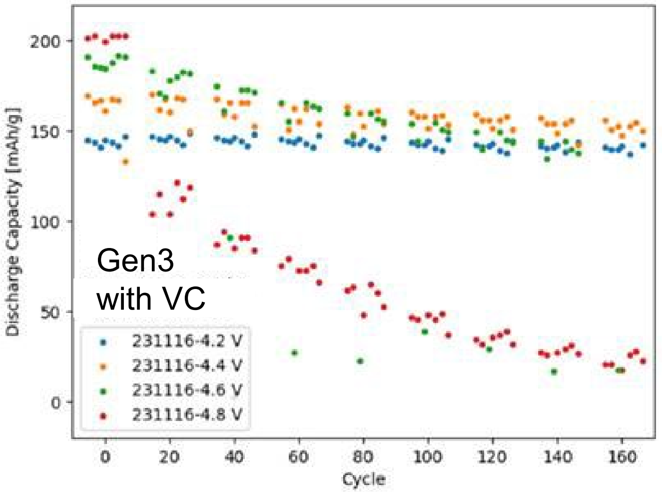
Automated coin cell assembly robot

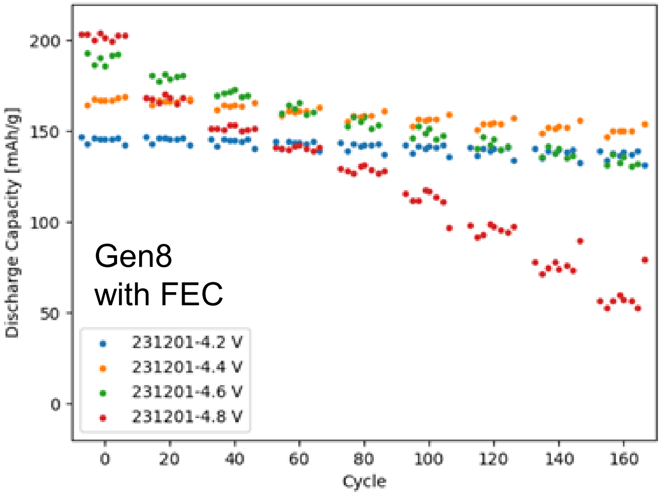
- Assembly of 32 coin cells per batch
- Automated electrode balancing
- Mixing of 32 electrolyte formulations

Automated coin cell cycling

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

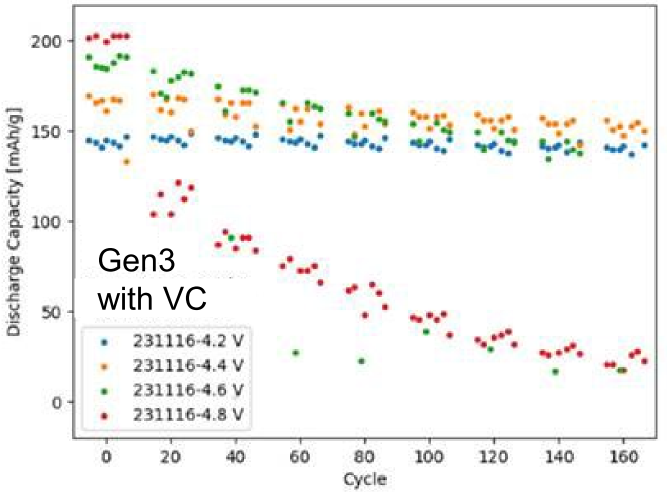
Proof-of-concept 10 generations à 32 cells

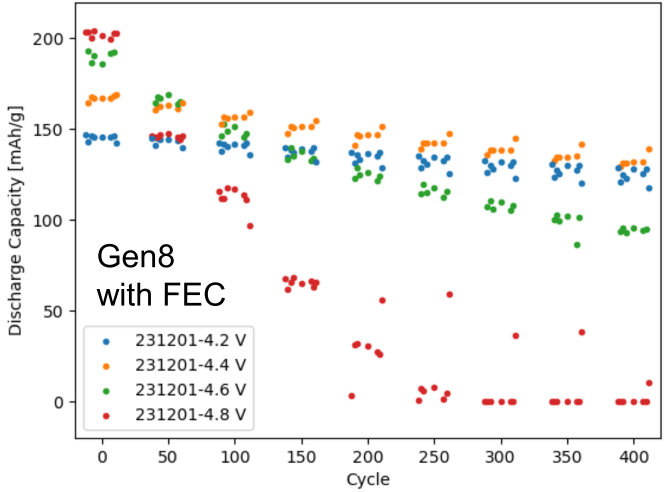




- Validation with NMC622 vs graphite cells in 1M $LiPF_6$ in EC:EMC 3:7
- Formation cycling at C/10, long-term cycling at 1C
- 32 cells split into groups of 8 cells cycled to different upper cut-off voltage

Proof-of-concept 10 generations à 32 cells





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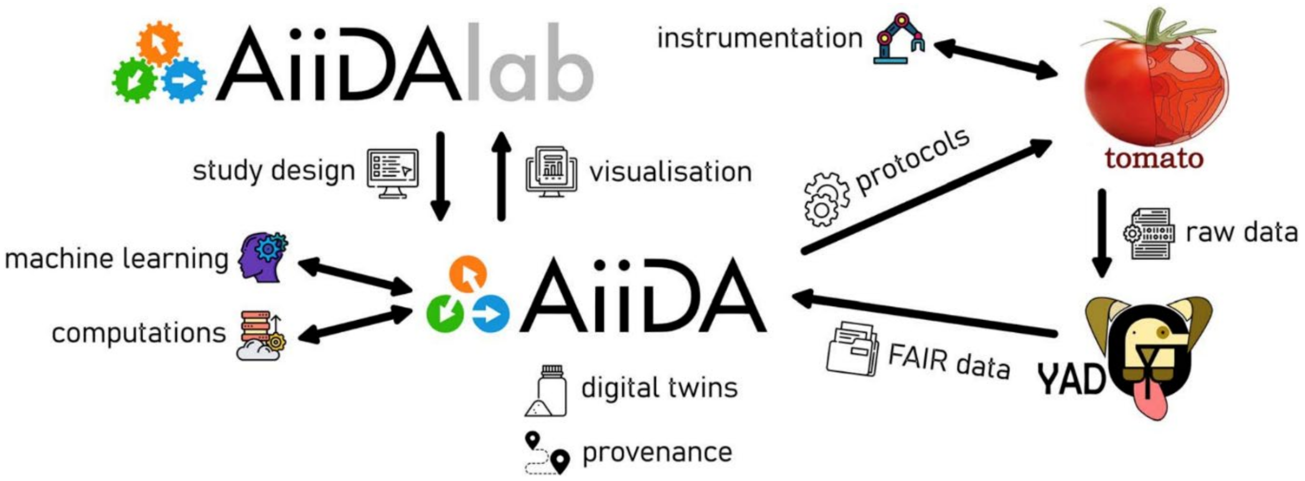
Automated workflow



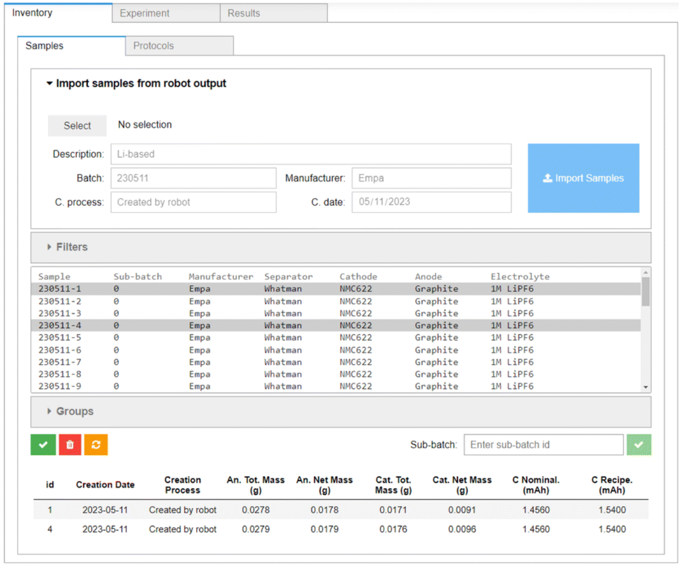
Automated Battery Cycling: Tomato manages and monitors battery cycling

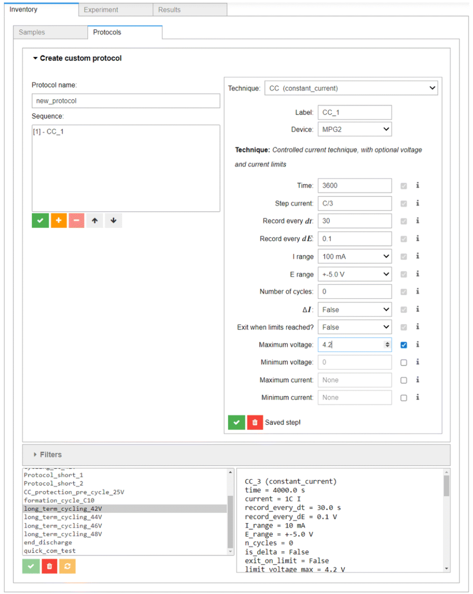
Integrated Workflow: Ensures seamless data flow from design to analysis

Real-time Monitoring: Maintains experiment accuracy and consistency

Graphical user interface: Easy to use

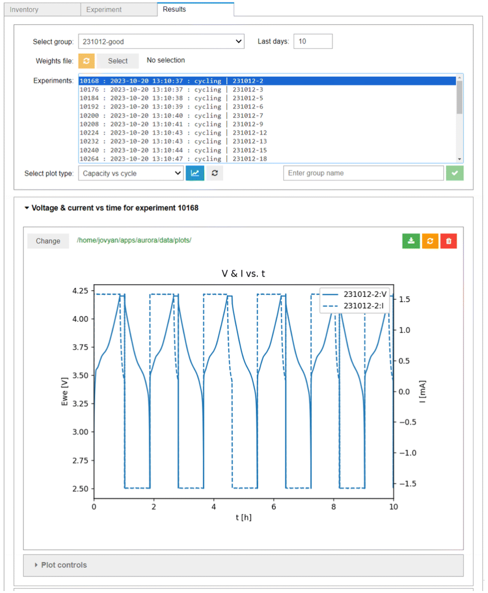
Aiida lab user interface

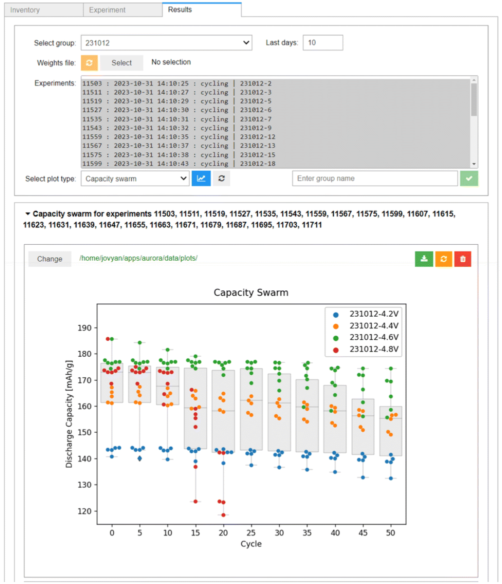




- Visualize metadata for each battery cell in a generation
- Specify cycling protocol for individual cells or groups of cells
- Batch submission and monitoring of cells during cycling

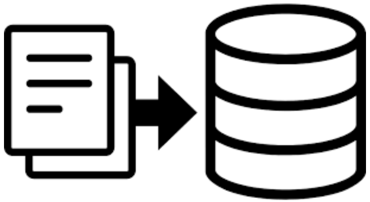
Aiida lab user interface





- 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

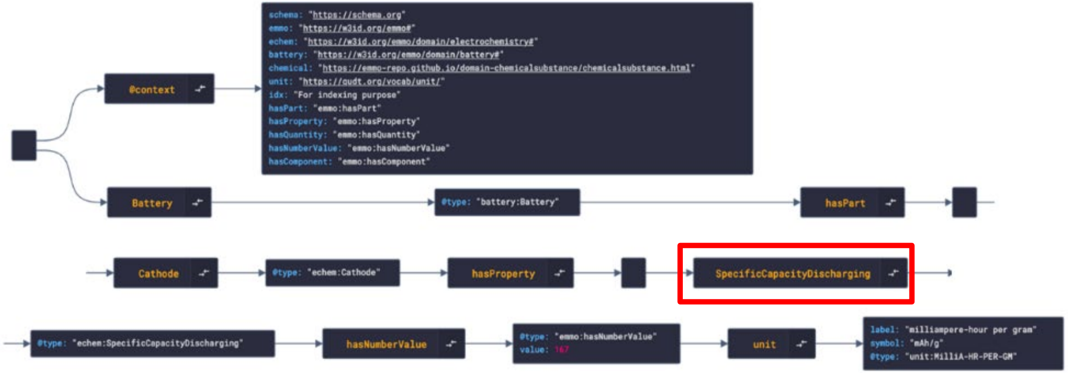
- (Meta)data are assigned a globally unique and persistent identifier
- (Meta)data are retrievable by their identifier via open, free protocols
- (Meta)data meet domain-relevant community standard

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

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Non-ontologized m

Data description	Dat valu
Cathode gravimetric discharge capacity	16


```json
{
  "@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-chemicalsubstance/chemicalsubstance.html",
    "unit": "https://qudt.org/vocab/unit/",
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    "hasProperty": "emmo:hasProperty",
    "hasQuantity": "emmo:hasQuantity",
    "hasNumberValue": "emmo:hasNumberValue",
    "hasComponent": "emmo:hasComponent"
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    "hasPart": {
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              }
            }
          }
        }
```
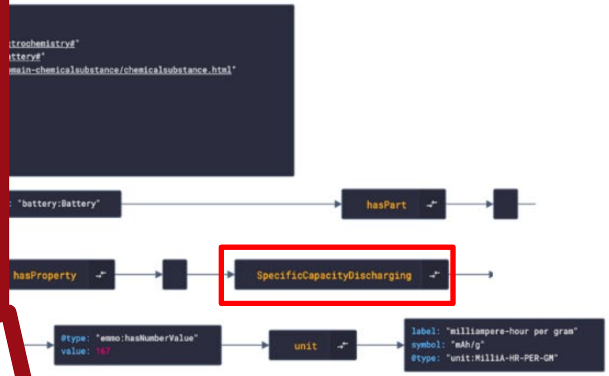


Manually ontologizing your data is laborious and prone to errors



- BattINFO ontolo ... ny
- BattINFO defi ... ps of battery-related concepts
- BattINFO ontol ... bles semantic searches

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

BattINFO Converter

- 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

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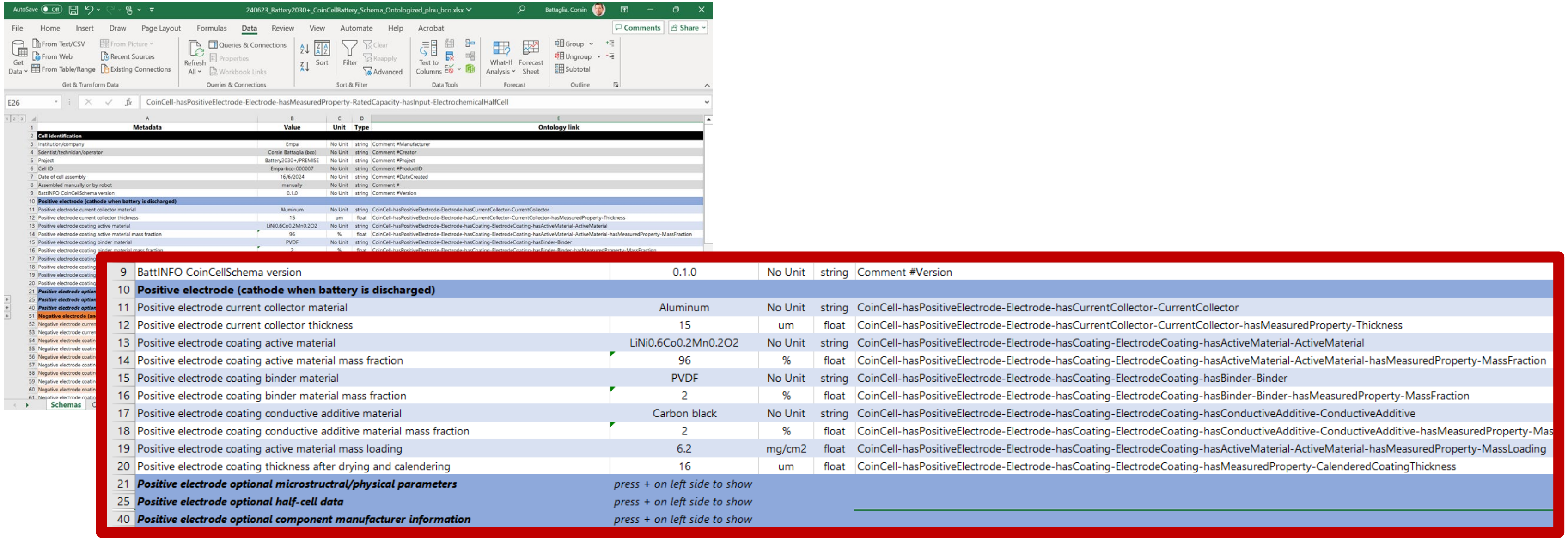
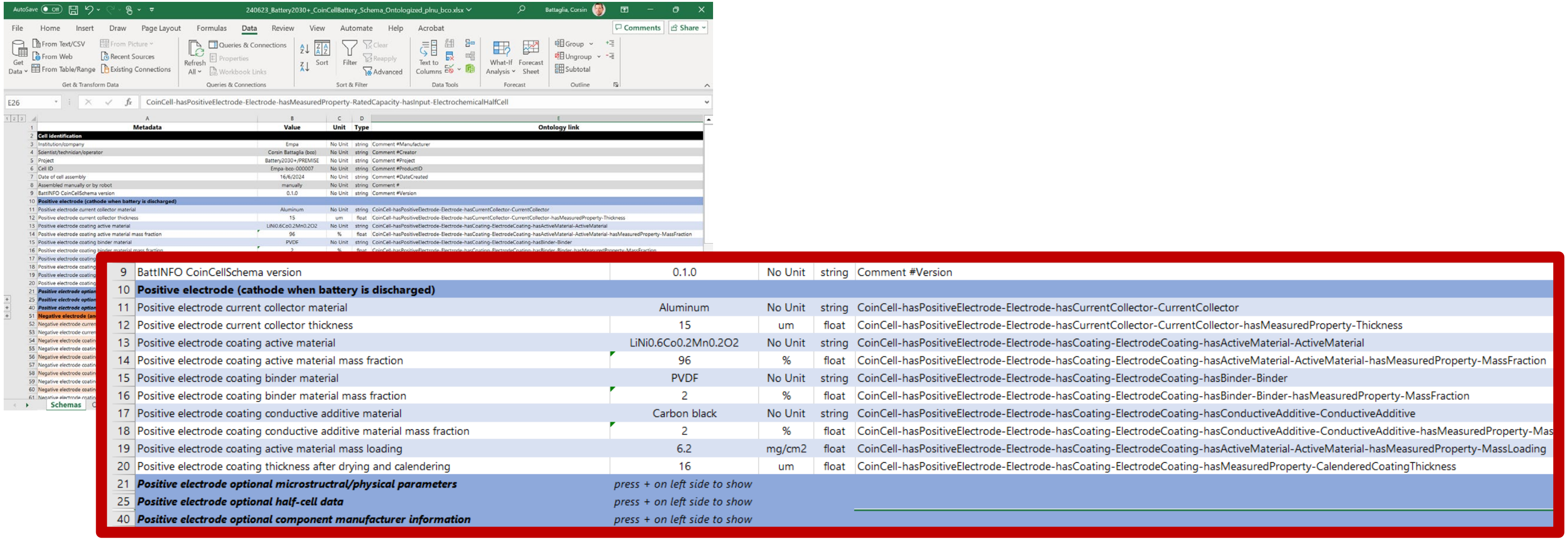


9	BattINFO CoinCellSchema version	0.1.0	No Unit	string	Comment #Version
10	**Positive electrode (cathode when battery is discharged)**				
11	Positive electrode current collector material	Aluminum	No Unit	string	CoinCell-hasPositiveElectrode-Electrode-hasCurrentCollector-CurrentCollector
12	Positive 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-Mas
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 calendering	16	um	float	CoinCell-hasPositiveElectrode-Electrode-hasCoating-ElectrodeCoating-hasMeasuredProperty-CalenderedCoatingThickness
21	***Positive electrode optional microstructral/physical parameters***	*press + on left side to show*			
25	***Positive electrode optional half-cell data***	*press + on left side to show*			
40	***Positive electrode optional component manufacturer information***	*press + on left side to show*			

- 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

Conclusions

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- **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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CHEMSPEED TECHNOLOGIES: Amira Abou-Hamdan, And team

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