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A bridge between trust and control: Computational workflows meet automated battery cycling

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Supporting information

This document is part of the Electronic Supporting Information archive for the above manuscript, available on Zenodo under DOI: 10.5281/zenodo.10020712. This document contains the following:

- A set of representative provenance graphs, automatically generated using AiiDA
- A set of supplementary screen shots of the ${\it Experiment}$ component of the <code>AiiDAlab-Aurora</code> user interface
- A figure containing the cell cycling results for all cells in the two studied batches

Further information and data is available on the above DOI. Please contact Peter Kraus for any queries about the ESI.

Automated AiiDA provenance graphs



Figure S1: An automatically generated provenance graph for an in-band battery cycling workflow. The central CyclingSequenceWorkChain node (orange) corresponds to the overall workflow. It is linked to three BatteryCyclerExperiment nodes (red), corresponding to the Protective charge, Formation cycles, and Long-term cycling protocols of the workflow. Note that the Exit Code for the Long-term cycling (upper BatteryCyclerExperiment node) is 150, denoting that the task was aborted via job monitoring; the other two BatteryCyclerExperiments have an Exit Code of 0, denoting successful completion. The green nodes correspond to the various Data nodes, required to assemble the CyclingSequenceWorkchain, and retrieve the raw data from the remote host running tomato.



Figure S2: An automatically generated provenance graph for an out-of-band battery cycling workflow. At the centre is a simple WorkChain node (orange), linked to a single CalcJob node (cf. Fig. S1). However, provided the Data nodes used to construct the WorkChain contain the relevant metadata information and instructions, AiiDA is able to process the out-of-band data into the same internal format as that used for in-band data.

Supplementary AiiDAlab-Aurora screenshots

	ct sam	nples							
→ Fi	Iters								
		Batch		Sub-batch		Manufacturer		Separator	
23	230511 [8]		4.2V [4.4V [0 [20]	4.2V [8] 4.4V [8] 0 [20]		[8]	Whatman [8]		
		Cathode		Anode		Electrolyte		Capacity (mAh)	
NA	NMC622 [8]		Graphi	Graphite [8]		PF6 [8]	1.456 [8]		
Ву	y group	all-samples		```	From:	mm/dd/yyyy	To:	mm/dd/yyyy	
		c 1	<u></u>						
Sam	pies:	Sample 230511-1	Sub-batch 4.2V	Manufacturer Empa	Separator Whatman	Cathode NMC622	Anode Graphite	Electrolyte 1M LiPF6	
	~	230511-2	4.2V	Empa	Whatman	NMC622	Graphite	1M LiPF6	
		230511-3	4.2V	Empa	Whatman	NMC622	Graphite	1M LiPF6	
	~	230511-4	4.2V 4.2V	Empa	Whatman	NMC622 NMC622	Graphite	1M LIPF6 1M LiPF6	
		230511-6	4.2V	Empa	Whatman	NMC622	Graphite	1M LiPF6	
		230511-7	4.2V	Empa	Whatman	NMC622	Graphite	1M LiPF6	
		250511-8	4.20	Спра	Wild Cliidi	NPICO22	draphice	IN LIFFO	
Sele	cted [.]	Sample	Sub-batch	Manufacturer	Separator	Cathode	Anode	Electrolvte	
0010	otou.	230511-1	4.2V	Empa	Whatman	NMC622	Graphite	1M LiPF6	
	*	230511-4	4.2V	Empa	Whatman	NMC622	Graphite	1M LiPF6	
	^								
								(
	of 1917-1	te ce la							
Bali	ct prot	tomato/monit	oring						
Sele	figure	comaco/monit	oning						
Sele	figure	nput							
Sele Conf Gene	figure erate i	nput	nlock when done?						

Figure S3: The *Select samples* section of the *Experiment* component of the AiiDA-Aurora user interface. This widget allows for filtering and selection of samples stored in the *Inventory*. The samples listed in the Selected section will be part of the workflow.

Inventory	Experiment	Results	
► Select sa	mples		
✓ Select pr	otocols		
Protocol:	cycling_1C_41V Protocol_short_1 Protocol_short_2 CC_protection_pre_cycc formation_cycle_C10 long_term_cycling_42V long_term_cycling_48V end_discharge CC_protection_pre_cycc formation_cycle_C10 long_term_cycling_42V end_discharge	le_25V le_25V	<pre>CC_3 (constant_current) time = 4000.0 s current = 1C I record_every_dt = 30.0 s record_every_dt = 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 limit_voltage_min = None limit_current_max = None limit_current_min = None limit_current_min = None CV_2 (constant_voltage) time = 2000.0 s voltage = 4.2 V record_every_dt = 30.0 s record_every_dt = 30.0 s</pre>
			C
► Configure	e tomato/monitoring		
▶ Generate	input		
	Unlock when	done?	
Experiment gr	oup label: Enter a group la	abel (default: yymmdd-hhm	mss)
36	Reichup-0.21C2	· · ·	

Figure S4: The *Select protocols* section of the *Experiment* component of the AiiDA-Aurora user interface. This widget allows for selection of protocols from the *Inventory*. The protocols will be executed in the order as listed in the Selected section.

Select	samples		Results					
	oumproo							
Select	protocols							
Config	jure tomato/m	onitoring						
 Genera 	ate input							
Samp	oles							
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
	localor lorina	tion_cyc iong_te	erm_cy end_	discharg v	erbosity: IN	FO		
CC_3 time curre recol recol I_rau E_rau	<pre>(constant_c = 4000.0 s ent = 1C I rd_every_dt rd_every_dt nge = 10 mA nge = +-5.0</pre>	urrent) = 30.0 s = 0.1 V	erm_cy	discharg v f p	erbosity: IN requency: 72 refix: snaps	FO 90 hot		
CC_3 time curra recol I_rau E_rau n_cyu is_du exit	<pre>(constant_c = 4000.0 s ent = 1C I rd_every_dt nge = 10 mA nge = +-5.0 v cles = 0 elta = False on limit =</pre>	urrent) = 30.0 s = 0.1 V V False	rm_cy	dischargi v f P	erbosity: IN requency: 72 refix: snaps lonitors	FO 90 hot		
CC_3 time curre recoi I_rai n_cyu is_de exit_ limi limi limi cV 2	<pre>(constant_c = 4000.0 s ent = 1C I rd_every_dE nge = 10 mA nge = +-5.0 cles = 0 elta = False _on_limit = t_voltage_ma t_ourrent_ma t_current_ma</pre>	<pre>urrent) = 30.0 s = 0.1 V V False x = 4.2 V n = None x = None n = None oltage)</pre>	rm_cy	discharge v f p P N N n r c t c	erbosity: IN requency: 72 refix: snaps lonitors ame: capacit efresh_rate heck_type = hreshold = 0 onsecutive_c	FO 20 hot 9 = 7200 discharge_ca .8 ycles = 3	pacity	
CC_3 time curry recou I_rau E_rau n_cyy is_dv exit limi limi limi CV_2 time	<pre>(constant_c = 4000.0 s ent = 1C I rd_every_dt nge = 10 mA nge = +-5.0 cles = 0 elta = False _on_limit = t_voltage_ma t_voltage_mi t_current_ma t_current_mi (constant_v = 2000.0 s</pre>	<pre>urrent) = 30.0 s = 0.1 V V False x = 4.2 V n = None x = None n = None oltage)</pre>	rm_cy	discharge v f p P V N N C t t c	erbosity: IN requency: 72 refix: snaps lonitors ame: capacit efresh_rate heck_type = hreshold = 0 onsecutive_c	FO po hot y = 7200 discharge_ca .8 y y y y y y y y y y y y y	pacity	
CC_3 time curry recou I_rau E_rau n_cyy is_dd exit limi limi limi limi CV_2 time volt	<pre>(constant_c = 4000.0 s ent = 1C I rd_every_dt nge = 10 mA nge = +-5.0 cles = 0 elta = False _on_limit = t_voltage_ma t_voltage_mi t_current_ma t_current_mi (constant_v = 2000.0 s age = 4.2 V good!</pre>	<pre>urrent) = 30.0 s = 0.1 V V False x = 4.2 V n = None x = None n = None oltage)</pre>	rm_cy	discharge p p V m r c t c	erbosity: IN requency: 72 refix: snaps lonitors ame: capacit efresh_rate heck_type = hreshold = 0 onsecutive_c	FO po hot y = 7200 discharge_ca .8 ycles = 3	pacity	
CC_3 time curry recoor I_ran E_ran n_cyu is_dd exit_ limi limi limi CV_2 time volta	<pre>(constant_c = 4000.0 s ent = 1C I rd_every_dT nge = 10 mA nge = +-5.0 cles = 0 elta = False _on_limit = t_voltage_ma t_current_ma t_current_ma t_current_mi (constant_v = 2000.0 s age = 4.2 V good!</pre>	<pre>urrent) = 30.0 s = 0.1 V V False x = 4.2 V n = None x = None n = None oltage) Unlock when doi </pre>	ne?	discharge v f p V N n r c t c	erbosity: IN requency: 72 refix: snaps lonitors ame: capacit efresh_rate heck_type = hreshold = 0 onsecutive_c	FO 20 hot = 7200 discharge_ca .8 ycles = 3	pacity	
CC_3 time curry recoin recoin I_ran E_ran n_cyy is_du exit limi limi limi limi CV_2 time volt; All	<pre>(constant_c = 4000.0 s ent = 1C I rd_every_dt nge = 10 mA nge = +-5.0 cles = 0 elta = False _on_limit = t_voltage_ma t_voltage_mi t_current_ma t_current_mi (constant_v = 2000.0 s age = 4.2 V good!</pre>	urrent) = 30.0 s = 0.1 V V False x = 4.2 V n = None x = None n = None oltage) Unlock when dor Enter a group labe	ne?	discharge v f p p V N v t dd-hhmmss)	erbosity: IN requency: 72 refix: snaps lonitors ame: capacit efresh_rate heck_type = hreshold = 0 onsecutive_c	FO 20 hot 9 7200 discharge_ca .8 ycles = 3	pacity	

Figure S5: The *Generate input* section of the *Experiment* component of the AiiDA-Aurora user interface. This widget allows the user to review the selected samples as well as protocols and their monitoring settings prior to submission via AiiDA.

Complete cell cycling results



Figure S6: A comparison of the capacity degradation of all cells in the two studied cell batches. The colour of the swarm plots denotes batch of the cells. The data from the 230511 batch (blue) represents out-of-band data, as it has been imported into AiiDA from EC-Lab. The data from the 231012 batch (orange) has been gathered in-band, using an AiiDA workflow. The box plots show the statistics for all cells plotted. The behaviour of the cells cycled up to 4.2 V (upper left), 4.4 V (upper right), as well as 4.6 V (lower right) is consistent between the two batches. However, the cells cycled up to 4.8 V start at a vastly different capacity (~175 mAh/g for the 231012 batch, vs ~195 mAh/g for 230511), and their capacity degradation also seems to occur at different rates, with all cells in the 231012 batch (orange) stopped by the job monitor within 20 cycles. Note that for the batch 231012 (orange), only 25 out of the 32 assembled cells are shown, as 7 cells have failed before the first cycle, due to an assembly failure or a software error.