Coal as Value-Added for Lithium Battery Anodes

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Project Overview

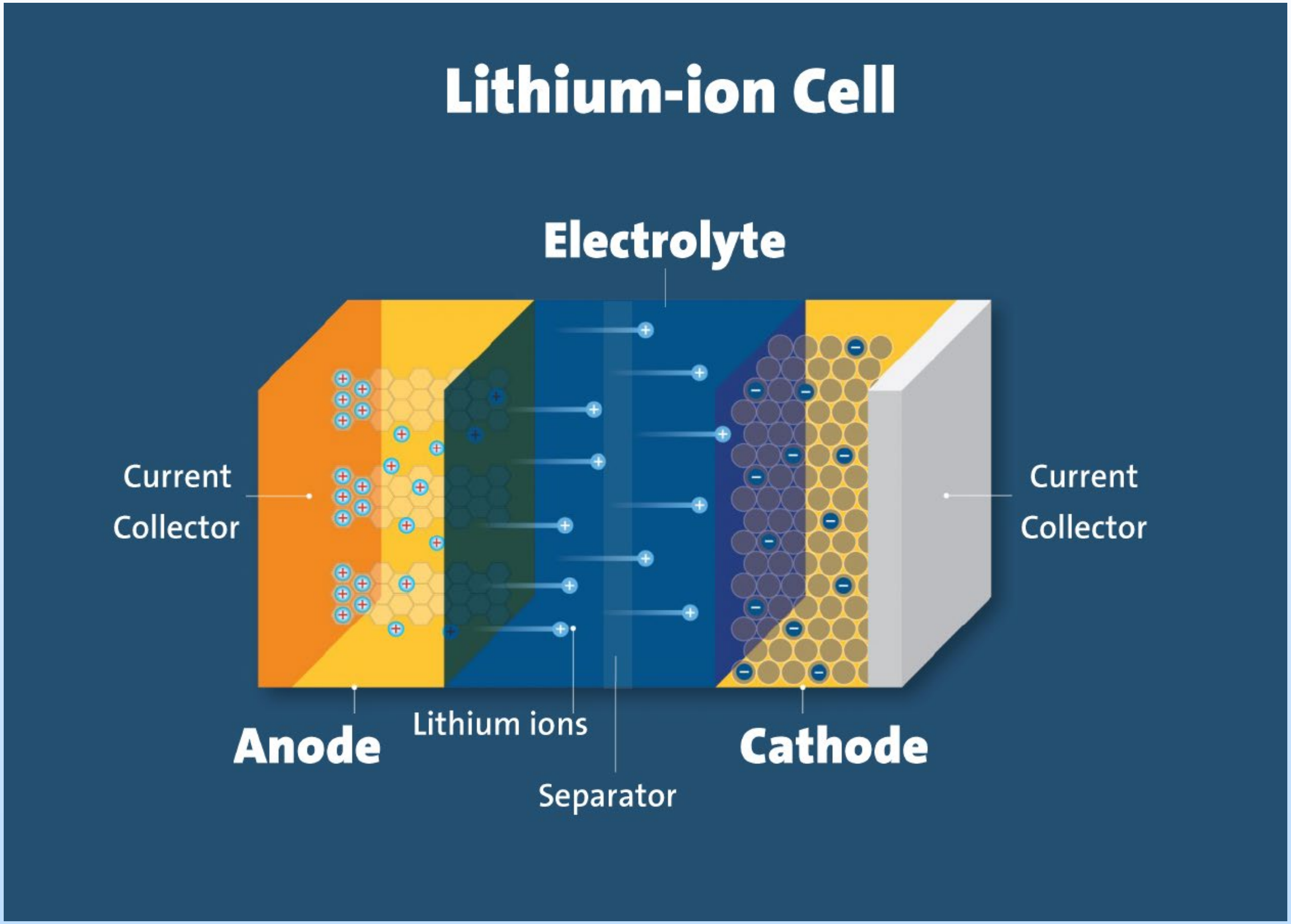
- Principal Investigator: Walter Sherwood, Ph.D.
- Lead Engineer: Kyle Marcus
- Funding
  - Federal = $749,942
  - Non-Federal = $187,500
  - Total Project = $937,442
- Period of Performance: 5/1/20-4/30/23
- Vendor
  - Battery Innovation Center (BIC)

Project Objectives

- Develop various novel anode composites utilizing coal and SiOC that have a higher capacity than graphite for lithium-ion batteries
- Scale up production of Anode Powders to support cell testing and development
- Produce and test 18650 Cylindrical Cells Utilizing the chosen coal-based anode composite

TECHNOLOGY OVERVIEW

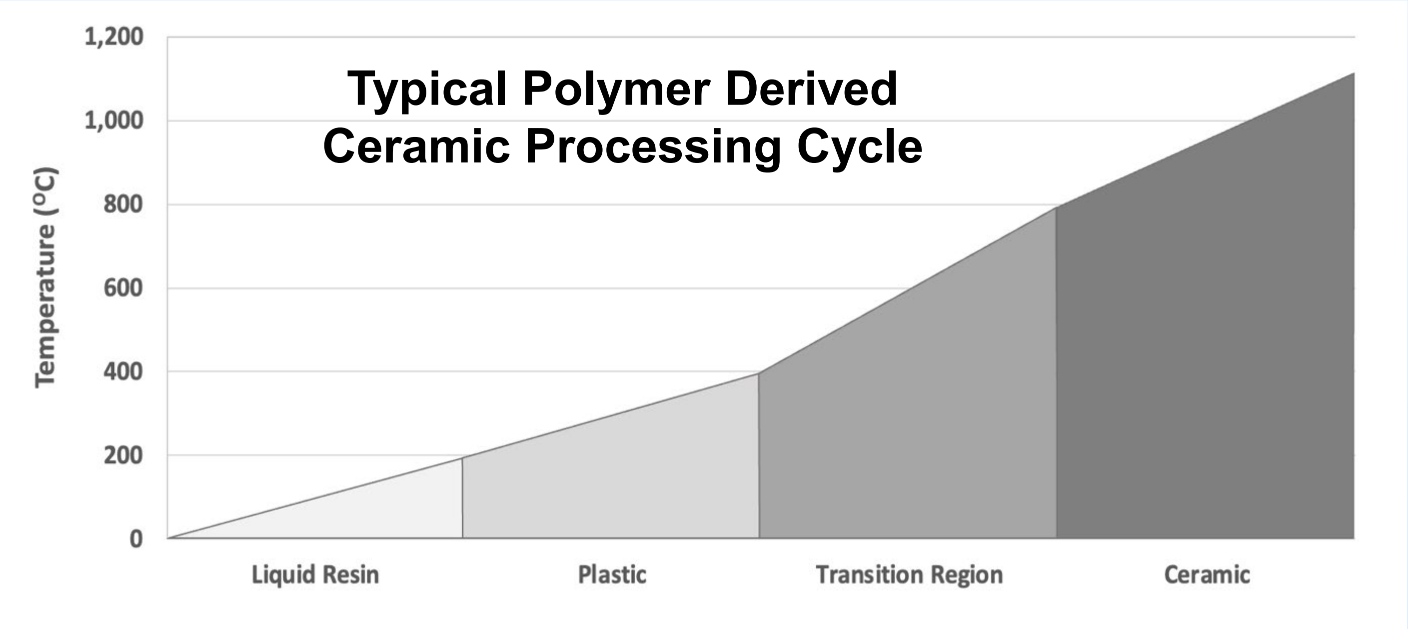
Lithium-Ion Battery Components



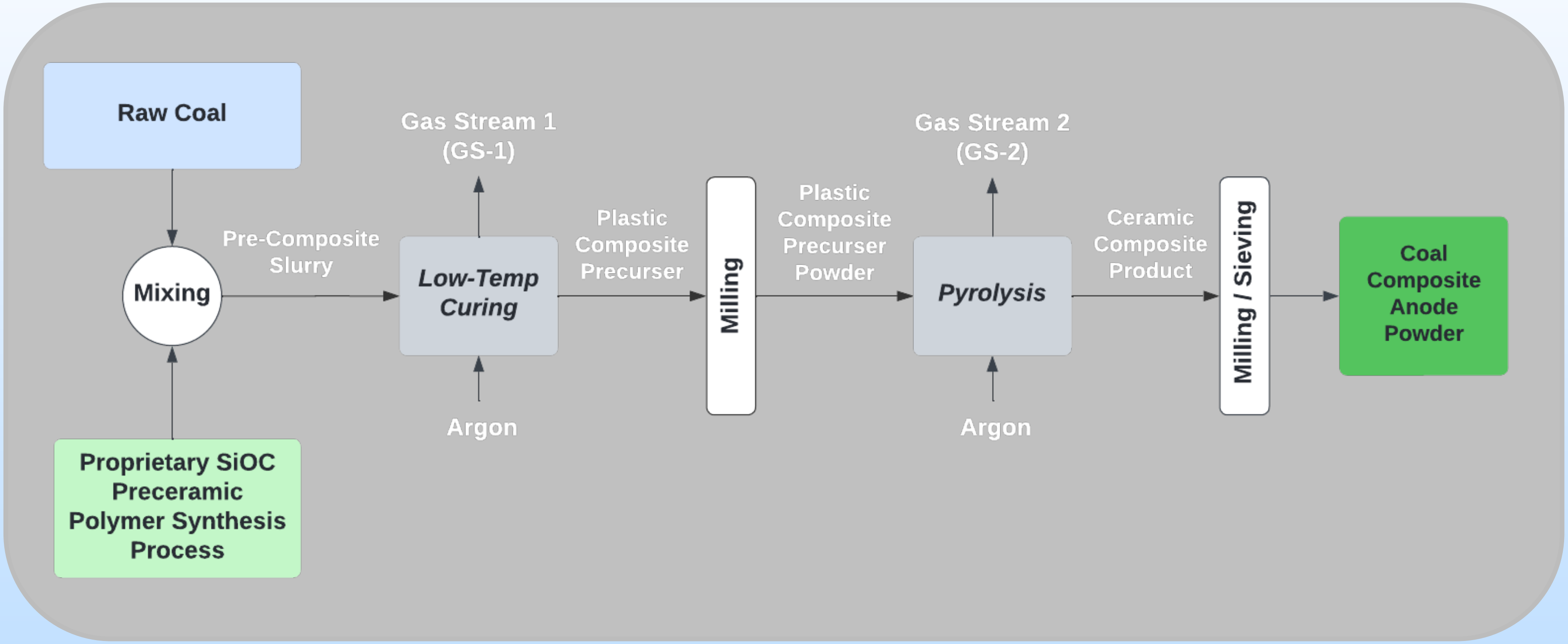
https://ul.org/research/electrochemical-safety/getting-started-electrochemical-safety/what-are-lithium-ion

The Technology

- Ceramic SiOC are called Polymer Derived Ceramic (PDC)
- Allow for drastic tuning of carbon, silicon & oxygen using simple, cost-effective techniques
- Processed below 1100^{o}C in inert gas
- Can be integrated with carbon or other fillers
- Crosslinked network of electrochemically active amorphous SiOC Matrix
- Can utilize abundant domestic resources such as coal

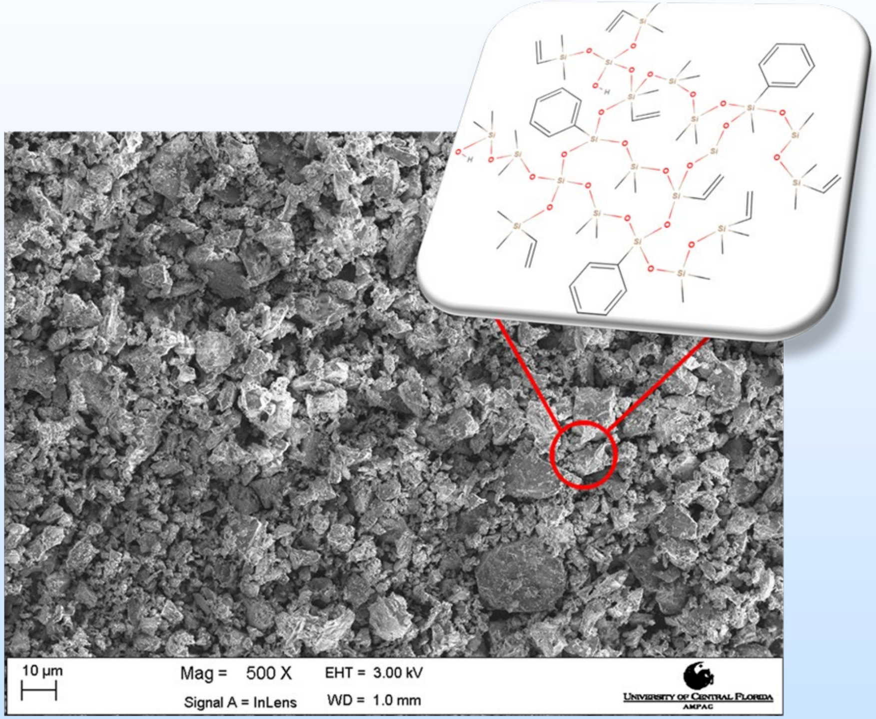


Simple, Scalable Process



Why Use PDC Composites as an Anode Material?

- High specific capacity compared to graphite
  - 500-800 mAh/g compared to 320-360 mAh/g
  - Graphite has nearly reached its theoretical capacity of 372 mAh/g
- The ceramic forming polymers can be integrated with impure carbon materials
- Low-cost and scalable methods to produce SiOC ceramics for use as lithium-ion battery anodes
- Cost competitive with traditional battery grade graphite, while producing higher intrinsic specific capacity



SEM/Schematic for Typical PDC

TECHNICAL APPROACH AND PROJECT SCOPE

Project Task Summary

Task 1.0 – Project Management and Planning (Years 1-3)

Task 2.0 – Formulation and Production of Test Samples (Years 1-2)

- *Formulate SiOC preceramic polymers*
- *Produce SiOC coal composite active material powders*
- *Fabricate battery cells for testing*

Task 3.0 – In-House Material Testing (Years 1-3)

- Test active materials in half and full coin cell orientation
- *Characterize active material powders*

Task 4.0 – Selection of Best SiOC and Coal Formulations (Year 2)

- *Down-select to best set of formulations*
- *Testing of best formulations in pouch cells (25 – 250 mAh)*

Task 5.0 – Scale-Up of Production (Year 3)

- Scale material to support large cell format builds

Task 6.0 – Production of Industrial Battery Prototypes (Year 3)

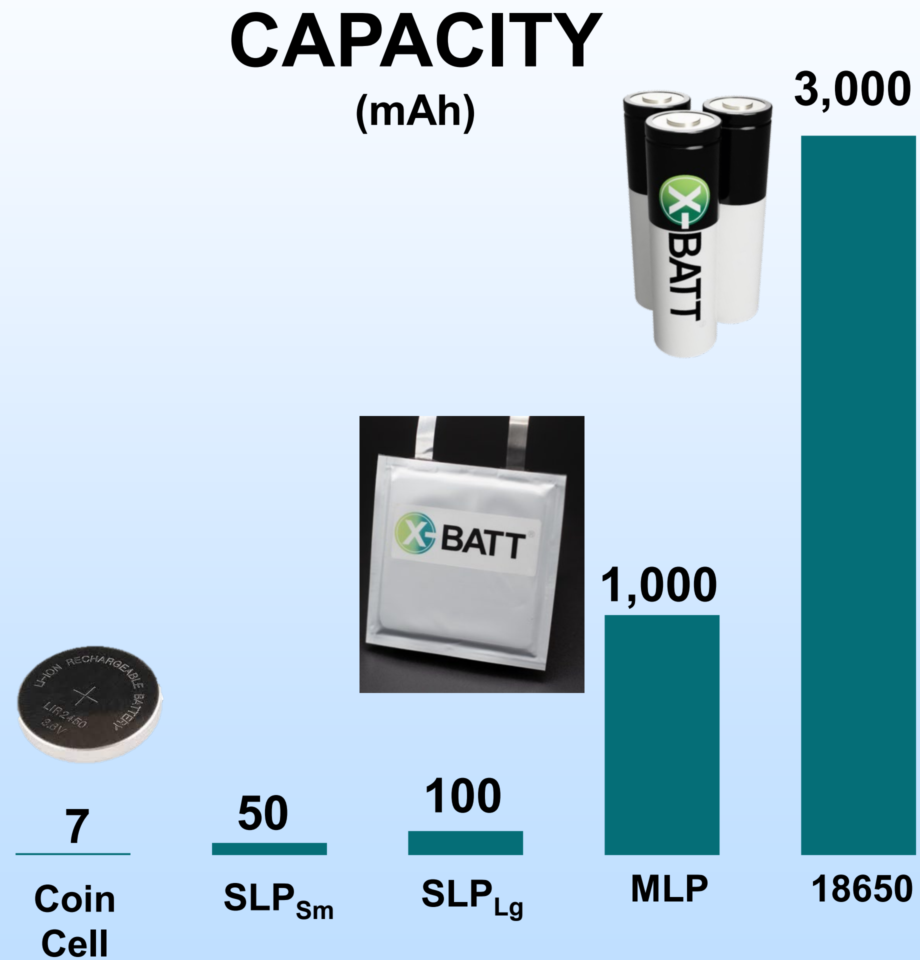
- Assemble and test 18650 cylindrical cells (3,000 – 5,000 mAh)

Milestone Log

Task / Subtask	Milestone Title & Description	Planned Completion	Actual Completion	Verification Method
2.3	Capability to test powders established	15 Jul 2020	**20 Jul 2020**	Results obtained for first slurry-bonded powder
4.1	Best coal material identified	30 Dec 2020	**28 Dec 2020**	Acceptable data from short-term half-cell testing of multiple resin formulations
4.2	Best overall composition identified	11 Aug 2021	**30 Aug 2021**	Favorable results from Battery Innovation Center testing
2.4	Production and testing capability for pouch cells established	29 Jul 2022	**18 Mar 2022**	Results obtained from testing of initial pouch cells
6.0	Initial set of industry-standard batteries produced	30 Dec 2022	**TBD**	Favorable initial test results from Battery Innovation Center testing
5.0	Pilot line for scaled-up material production established	28 Apr 2023	**TBD**	Demonstrated vendor production of 50 kg of material per week

Success Criteria

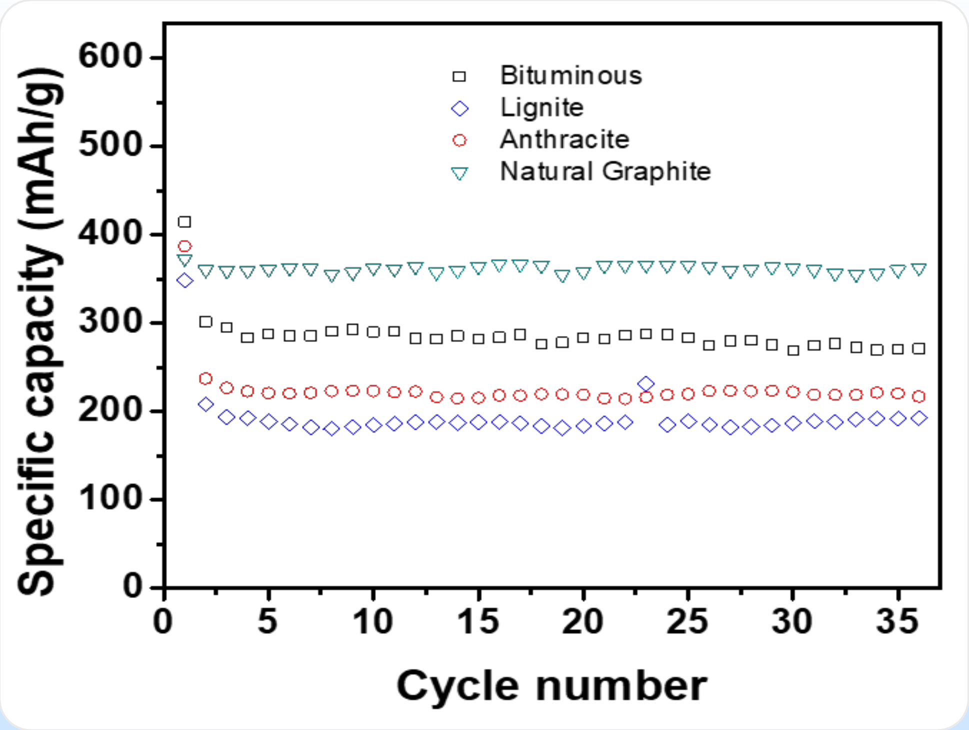
- Demonstration of anode performance in half coin cell of 600 to 900 mAh/g
- Demonstration of performance of full coin cell of 160 to 220 mAh/g
- Demonstration of 18650 cylindrical cell prototype industrial-grade battery performance of 3,000 to 5,000 mAh



PROGRESS & ACCOMPLISHMENTS

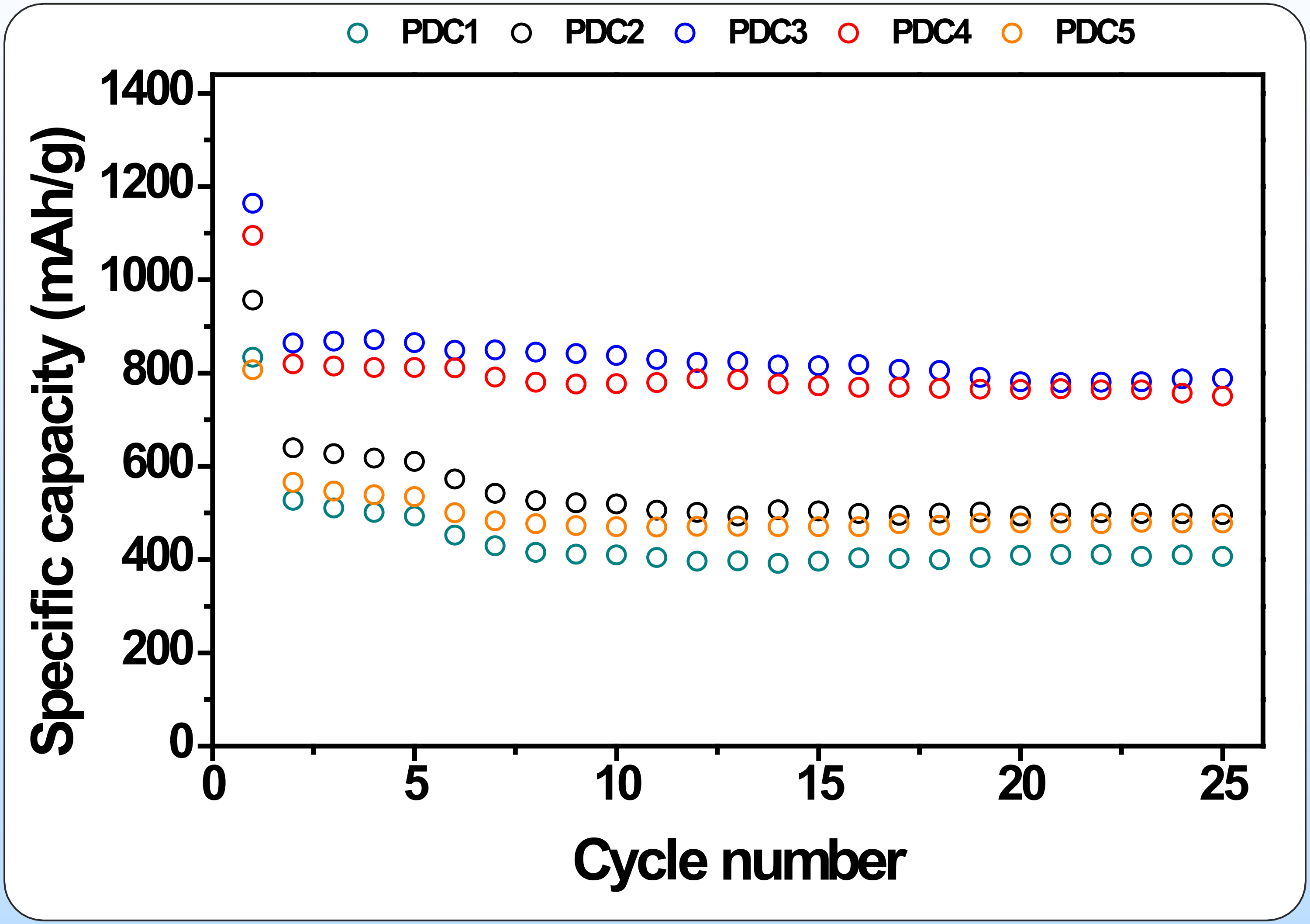
Coal Standalone Active Material

- Specific discharge capacity (mAh/g) comparing experimental Half-Cells to a Natural Graphite Control Half-Cell.
- Active Material: 100% coal heated to below 1100C under argon
- Half 2032-coin cells assembled and tested In-House



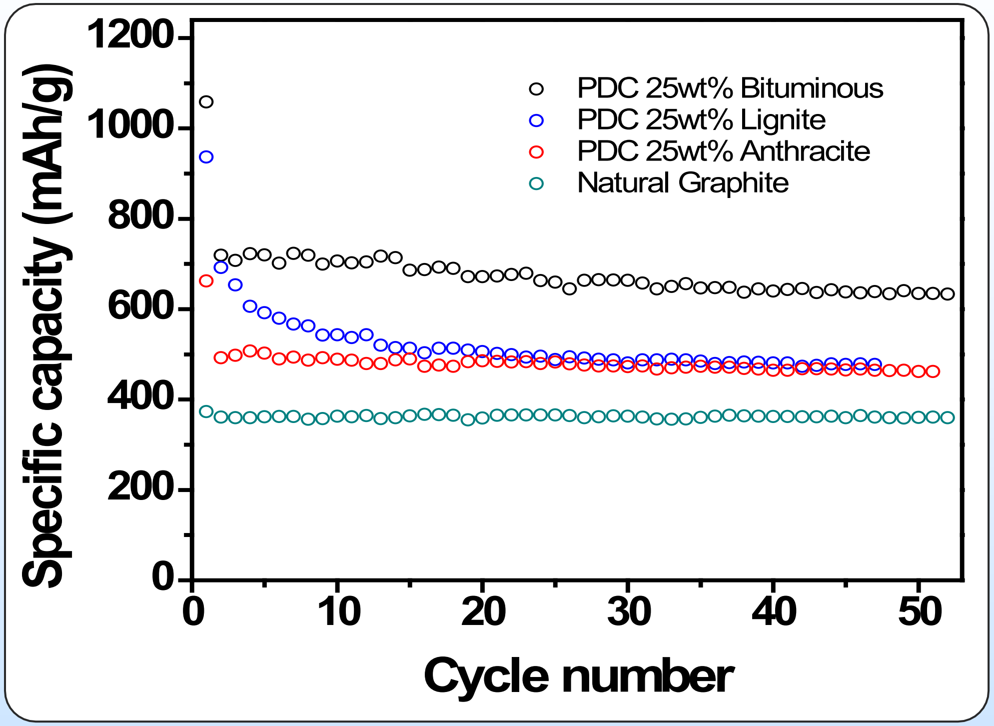
Material	1st Lithiation (mAh/g)	First Cycle Efficiency (%)	10th Lithiation (mAh/g)
Bituminous	414.6	71.4	290.0
Lignite	348.6	56.4	184.8
Anthracite	387.3	59.7	223.2
Natural Graphite	373.3	92.9	363.2

PDC Standalone Active Material



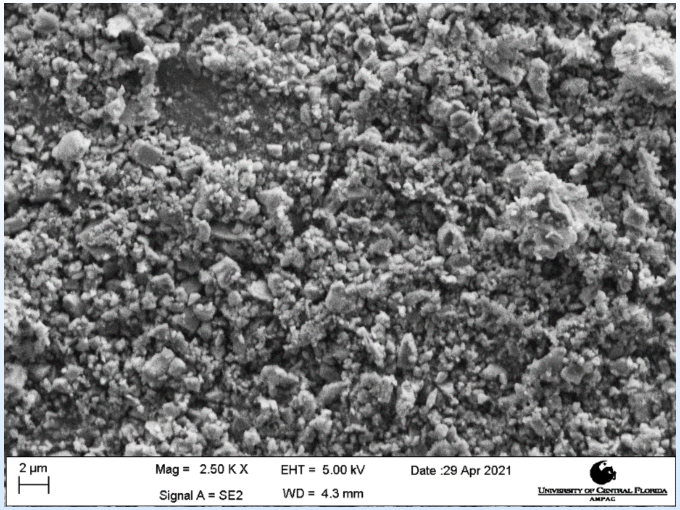
Coal + PDC Anode Composite Half Cell

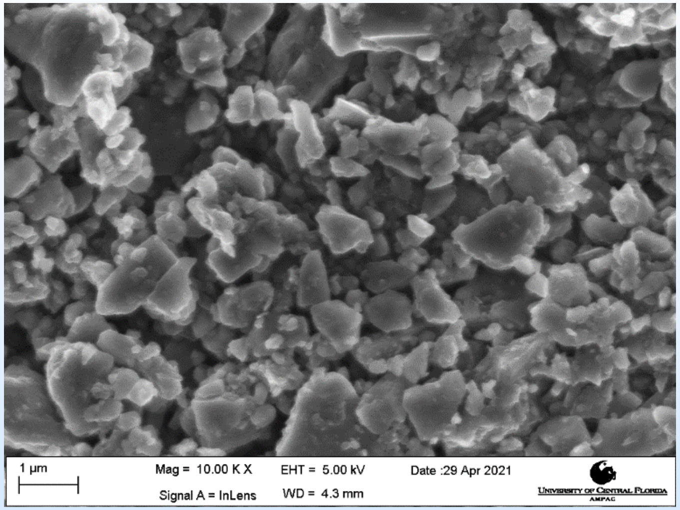
- Specific discharge capacity (mAh/g) comparing experimental Half-Cells to a Natural Graphite Control Half-Cell.
- Active Material: 25wt% coals and 75wt% SiOC resin.
- Half 2032-coin cells assembled and tested In-House



Material	1st Lithiation (mAh/g)	First Cycle Efficiency (%)	10th Lithiation (mAh/g)
Bituminous	1058.4	75.4	706.3
Lignite	936.3	73.8	543.1
Anthracite	662.3	72.6	489.2
Natural Graphite	373.3	92.9	363.2

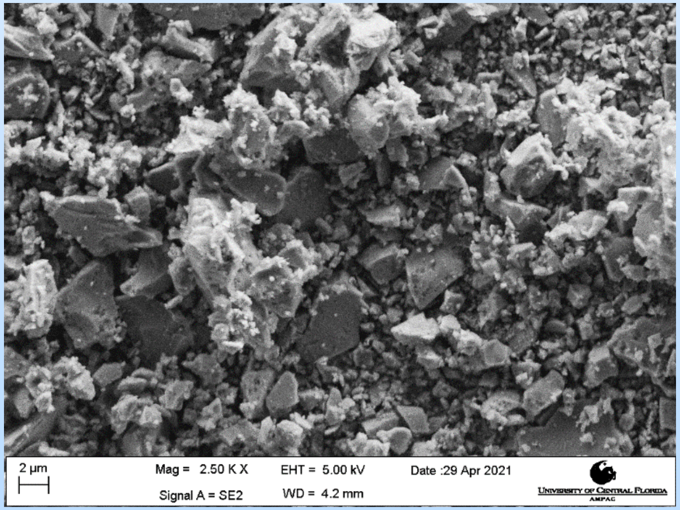
Active Material Morphology

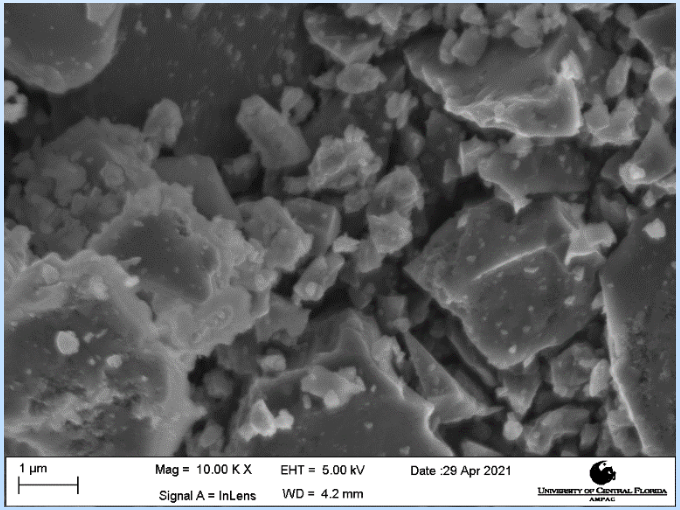




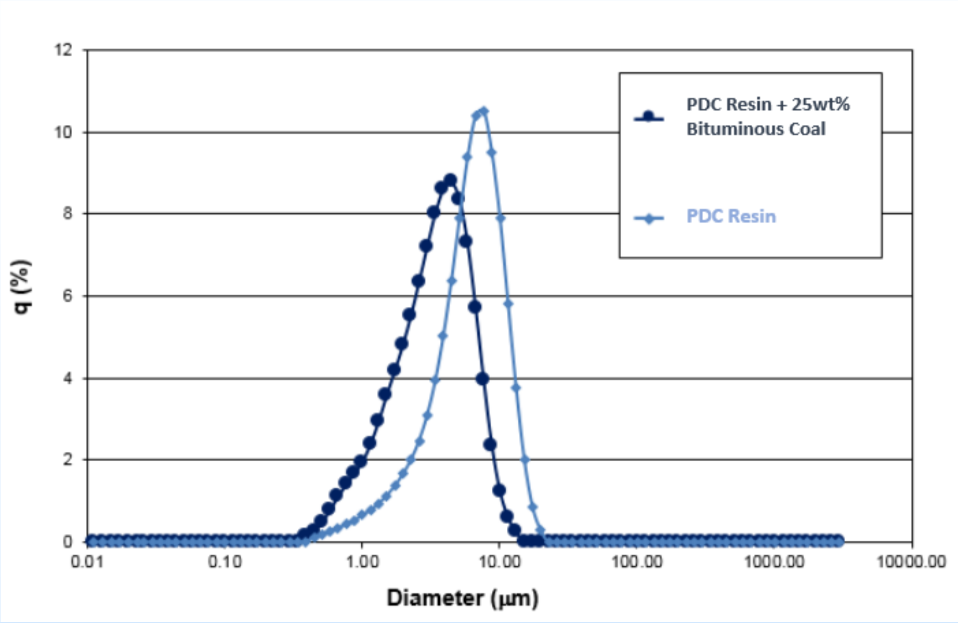
PDC + 25wt% Bituminous Coal

PDC





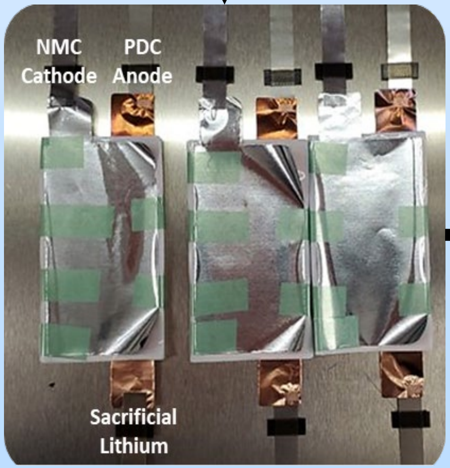
Active Material Powder Characterization

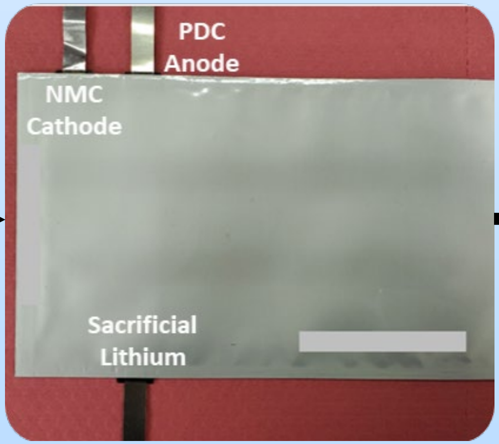


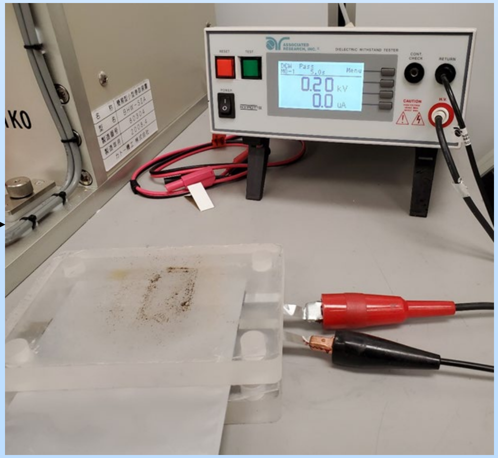
	ρ_{HE} (g/cm³)	BET Surface Area (m²/g)	MPV (cm³/g)	TOPV (cm³/g)	Mean (μm)	Mode (μm)	D_{10} (μm)	D_{50} (μm)	D_{90} (μm)
PDC + 25wt% Bituminous Coal	2.0932± 0.0021	19.7	0.0053	0.0506	3.59	4.17	1.12	3.25	6.47
PDC Resin	2.2077± 0.0011	9.1	0.0024	0.0363	6.29	7.15	2.18	5.96	10.77

Single-Layer Pouch (SLP) Cell Assembly

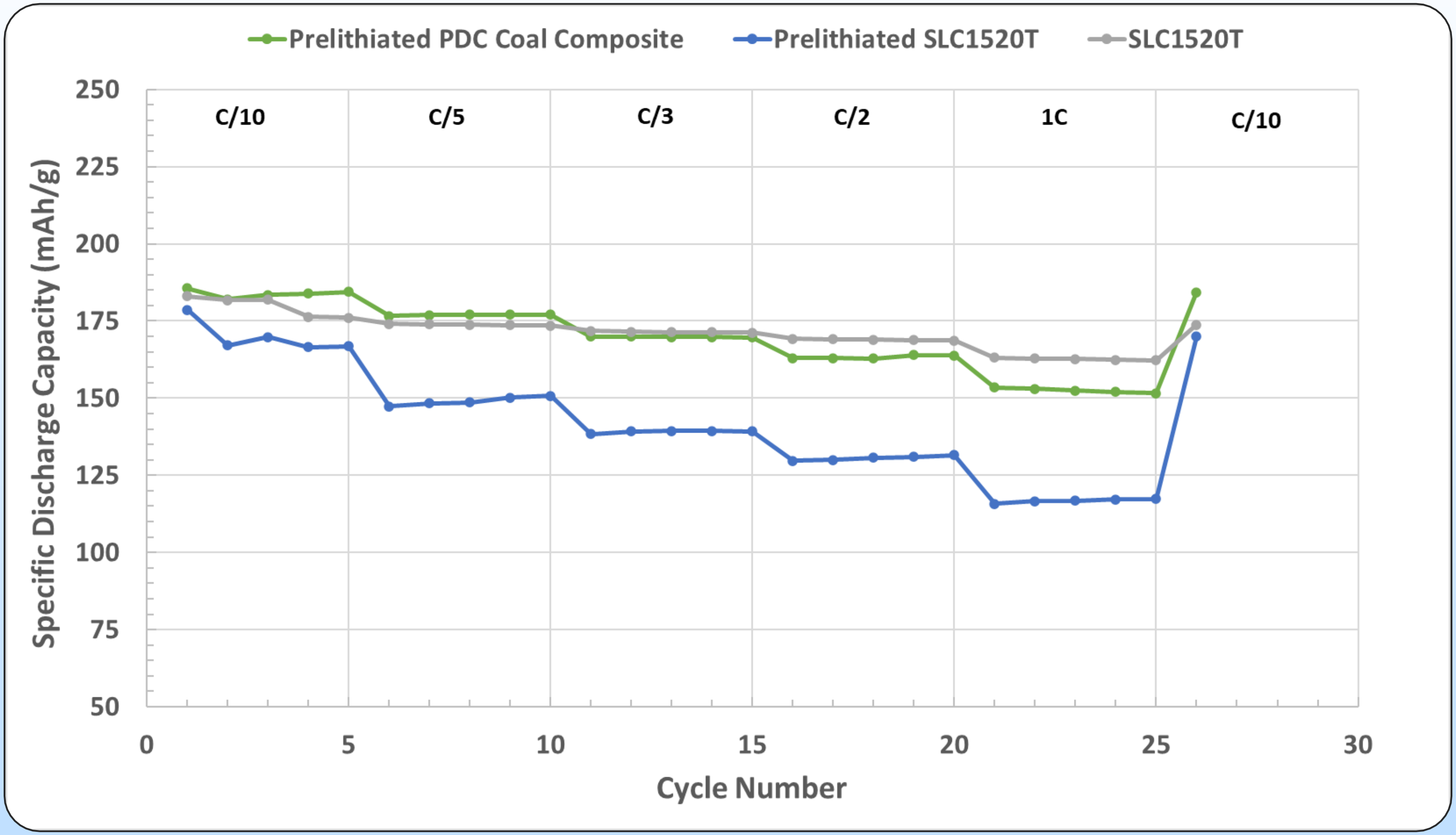
- Performed at the Battery Innovation Center in Indiana.
- 4.2 cm X 7.0 cm, 27 mAh cells
- PDC coal composite anode (PDC + 25wt% Bituminous Coal) or graphite vs NMC532 cathode
- For electrochemical prelithiation, cells are constructed tri-layer orientation.
- Anode / separator / sacrificial lithium plated Cu foil / separator / cathode
- Initial formation occurs between anode and lithium foil, lithium foil is removed then secondary formation and cycling between anode and cathode proceeds.



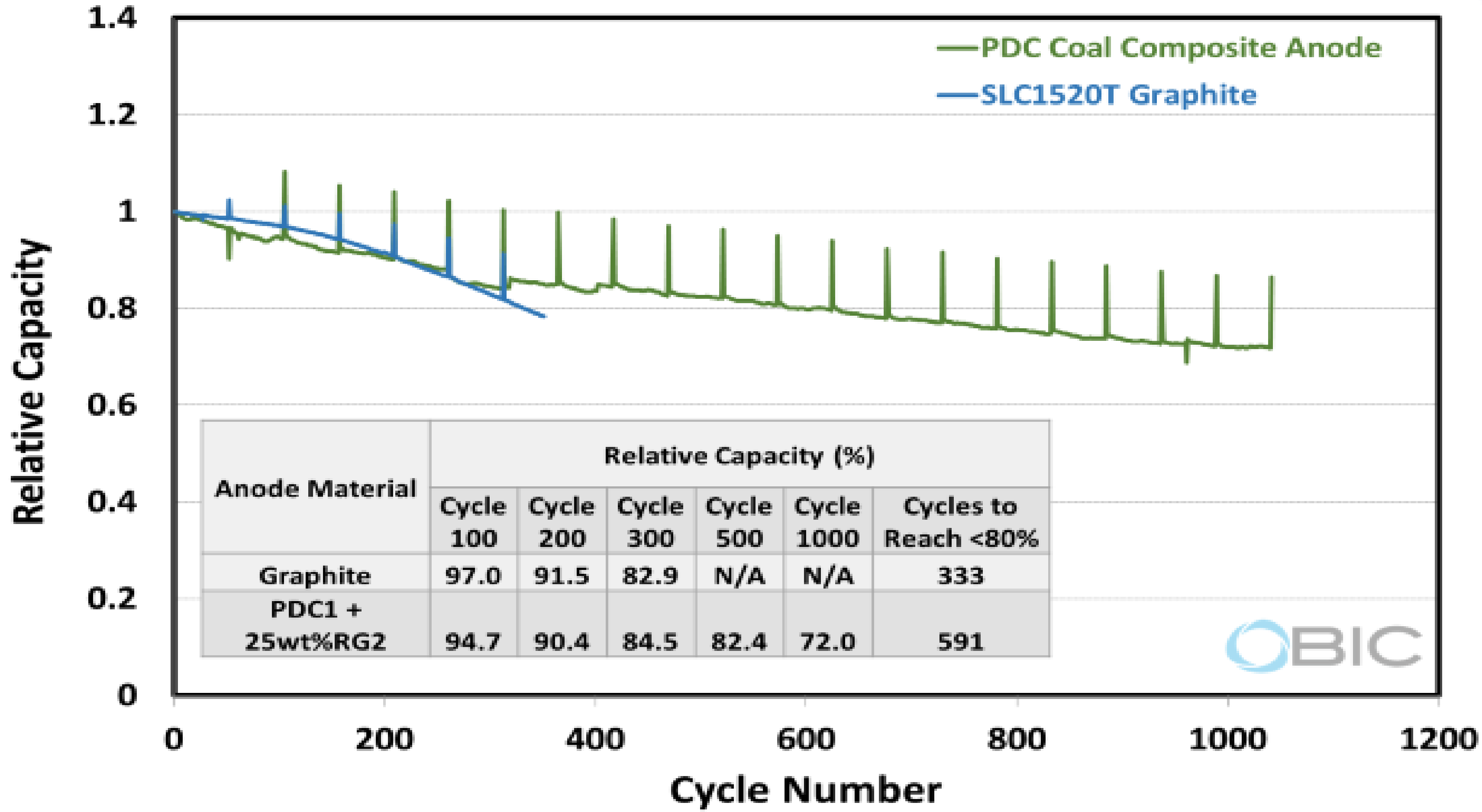




SLP Rate Performance Comparison

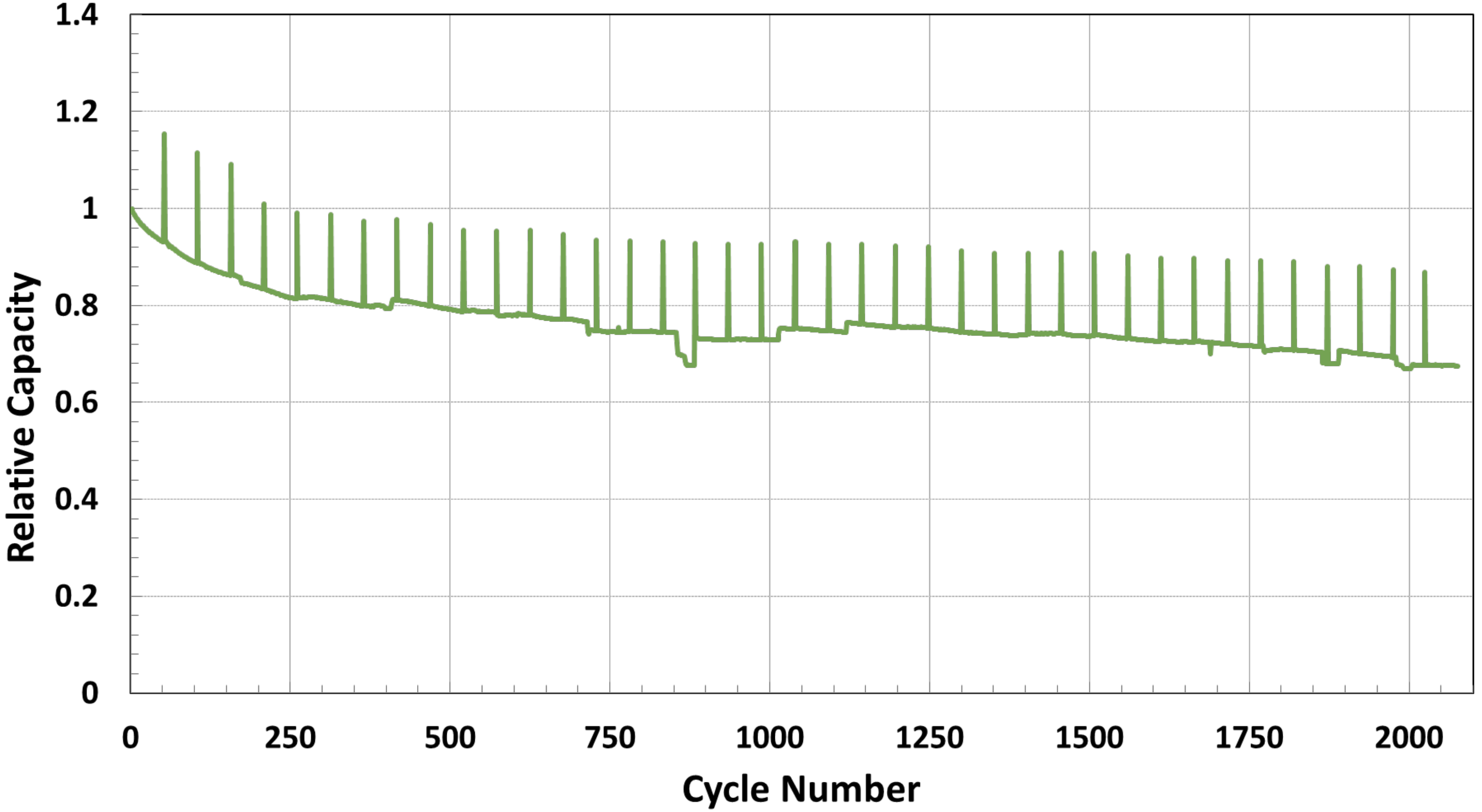


SLP Charge / Discharge Cycling Comparison

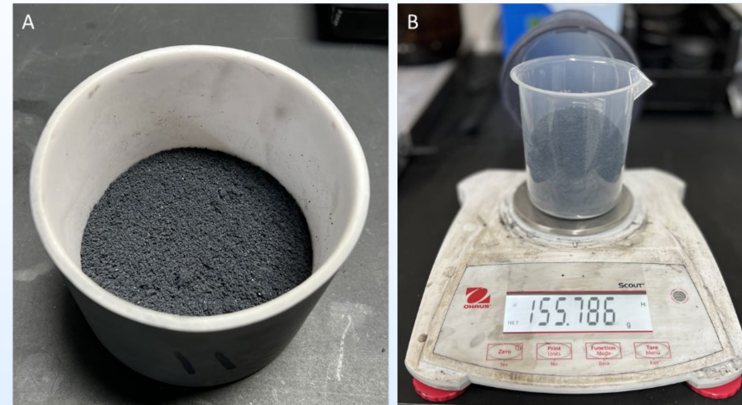


Anode Material	Relative Capacity (%)					
	Cycle 100	Cycle 200	Cycle 300	Cycle 500	Cycle 1000	Cycles to Reach <80%
Graphite	97.0	91.5	82.9	N/A	N/A	333
PDC1 + 25wt%RG2	94.7	90.4	84.5	82.4	72.0	591

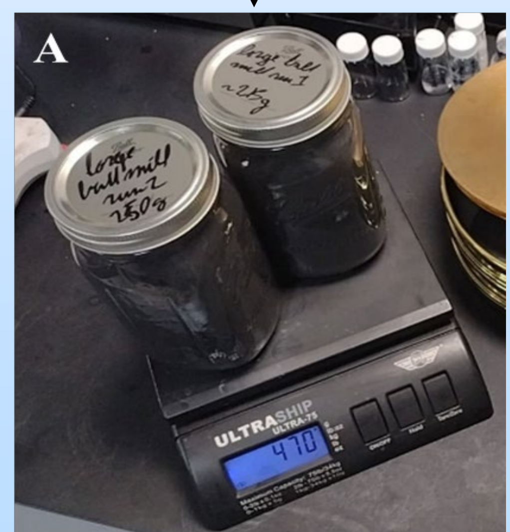
SLP Long-Term Cycling Performance



Our Next Steps



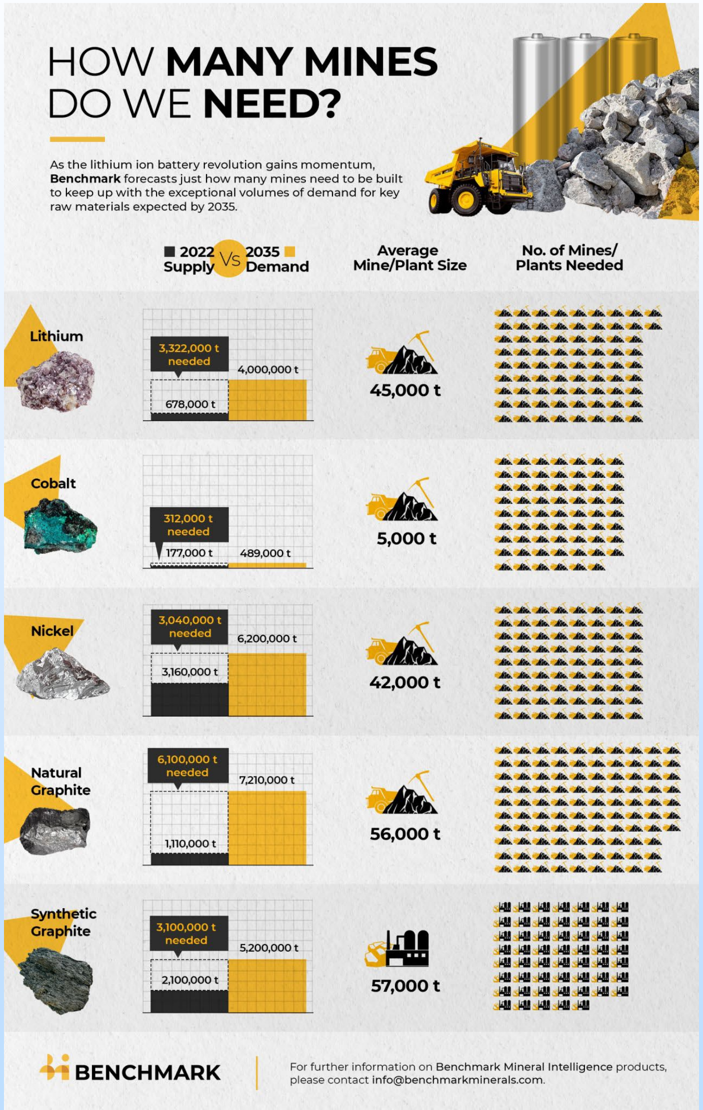
- Scale-Up of Powder
  - Beginning of Project: 10-20g
  - Currently: 500g
  - EOP: 10-50 Kg



- Scale-Up Test Cells
  - Beginning of Project: Coin Cell
  - Currently: BIC building SLP_{Lg} >100 mAh
  - EOP: 18650 Cylindrical cell

Why Coal Based Anodes Matter

- Adding coal to PDC anodes offers the following benefits:
  - Improves charge and discharge behavior
  - Decreases in nominal voltage
  - Increases FCE
  - Lowers overall material cost
  - SiOC PDC resin raws and selected coal is domestically sourced
  - Higher specific capacities than the theoretical value of graphite, requiring less overall material
  - CapEx required for this technology is very low compared to graphite manufacturing and other alternative anode technology
- By 2035, 150 graphite mines will be required to meet demand globally.



Summary

- Successful in creating a viable SiOC coal composite anode with higher specific capacity compared to battery grade graphite
- Tested active material performance in half coin cells, full coin cells, and full SLP cells at the BIC
- Forecasted to accomplish remaining milestones on time, including build and test of initial 18650 cylindrical cells
- Due to the lack of supply for battery grade graphite, coal anodes can offer a viable pathway to support the battery anodes supply chain.

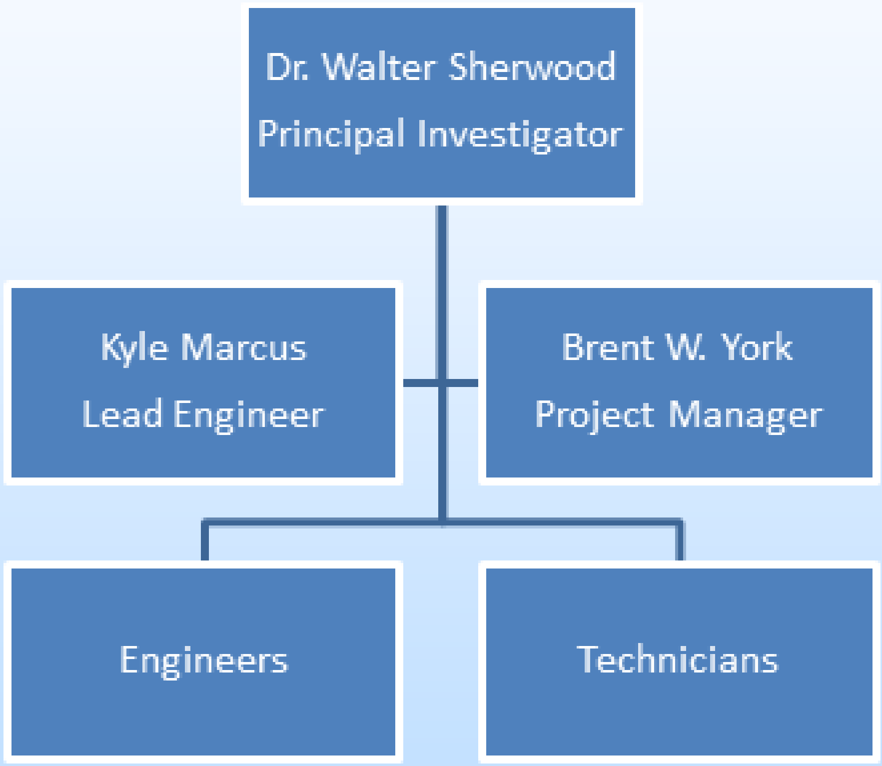
Acknowledgments

- NETL
  - Technology Manager - Joe Stoffa
  - Federal Project Manager – Christian Robinson
- The Battery Innovation Center
  - Advanced Battery Scientist - Scott Gray
  - Advanced Battery Manufacturing Team Lead - Wan Si Tang
- Semplastics Team

APPENDIX

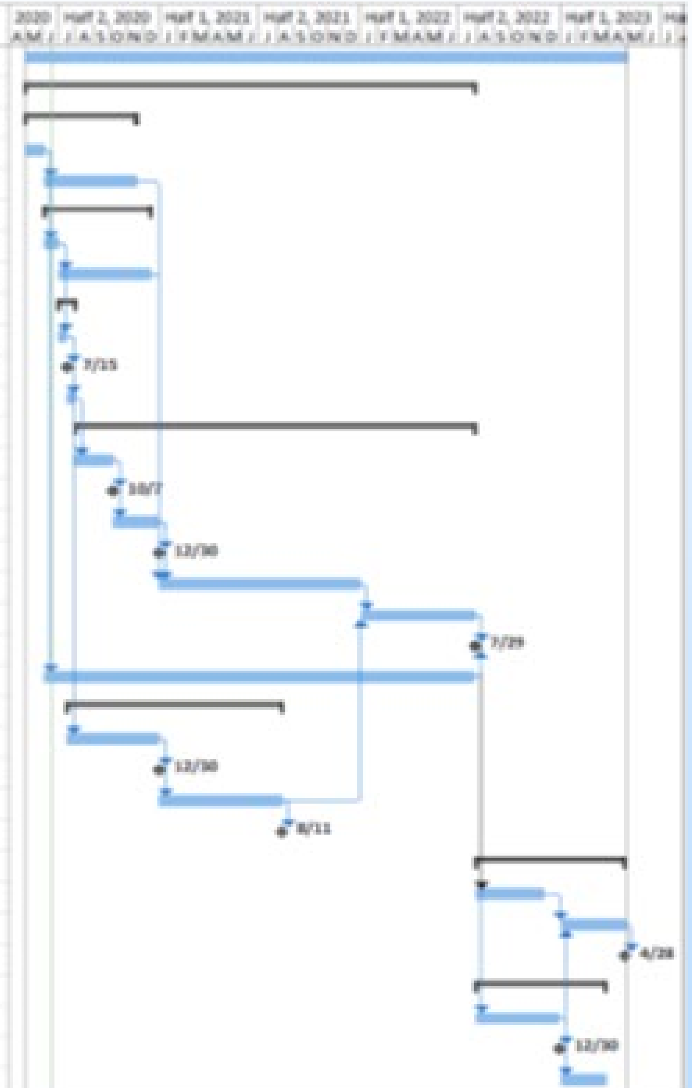
These slides will not be discussed during the presentation but are mandatory.

Organization Chart



Gantt Chart

ID	Task	Task Name	Duration	Start	Finish	Predecessors
1	**1.0**	**Project Management and Planning**	**784 days**	**Fri 5/1/20**	**Wed 5/3/23**	
2	**2.0**	**Formulation and Production of Test Samples**	**586 days**	**Fri 5/1/20**	**Fri 7/29/22**	
3	2.1	Formulate SiOC preceramic polymers	**144 days**	**Fri 5/1/20**	**Wed 11/18/2**	
4		Formulate initial SiOC preceramic polymers	24 days	Fri 5/1/20	Wed 6/3/20	
5		Refine SiOC preceramic polymers	120 days	Thu 6/4/20	Wed 11/18/2	4
6	2.2	Produce SiOC-coated coal powders	**139 days**	**Thu 6/4/20**	**Tue 12/15/20**	
7		Produce initial SiOC-coated coal powders	19 days	Thu 6/4/20	Tue 6/30/20	4
8		Refine SiOC-coated coal powders	120 days	Wed 7/1/20	Tue 12/15/20	7
9	2.3	Slurry-bond powders onto copper current collectors	22 days	Wed 7/1/20	Thu 7/30/20	
10		Produce and test first slurry-bonded powder	11 days	Wed 7/1/20	Wed 7/15/20	7
11		Capability to test powders established	0 days	Wed 7/15/20	Wed 7/15/20	10
12		Refine slurry-bonded powder production	11 days	Thu 7/16/20	Thu 7/30/20	10
13	2.4	Fabricate battery cells for testing	521 days	Fri 7/31/20	Fri 7/29/22	
14		Fabricate and test first half cell	49 days	Fri 7/31/20	Wed 10/7/20	12
15		Production and testing capability for half cells established	0 days	Wed 10/7/20	Wed 10/7/20	14
16		Fabricate and test first full cell	60 days	Thu 10/8/20	Wed 12/30/2	14
17		Production and testing capability for full cells established	0 days	Wed 12/30/2	Wed 12/30/2	16
18		Refine fabrication and testing of half and full coin cells	262 days	Thu 12/31/20	Fri 12/31/21	16,5,8
19		Fabricate and test initial pouch cells	150 days	Mon 1/3/22	Fri 7/29/22	18,25
20		Production and testing capability for pouch cells established	0 days	Fri 7/29/22	Fri 7/29/22	19,21
21	**3.0**	**In-House Material Testing**	**560 days**	**Thu 6/4/20**	**Wed 7/27/22**	**4**
22	**4.0**	**Selection of Best SiOC and Coal Formulations**	**280 days**	**Thu 7/16/20**	**Wed 8/11/21**	
23	4.1	Down-select to best set of formulations	120 days	Thu 7/16/20	Wed 12/30/2	10
24		Best coal material identified	0 days	Wed 12/30/2	Wed 12/30/2	23
25	4.2	Engage vendor for independent testing of best formulations	160 days	Thu 12/31/20	Wed 8/11/21	23
26		Best overall composition identified	0 days	Wed 8/11/21	Wed 8/11/21	25
27	**5.0**	**Scale-Up of Production**	**195 days**	**Mon 8/1/22**	**Fri 4/28/23**	
28		Produce initial pilot line design	90 days	Mon 8/1/22	Fri 12/2/22	20
29		Refine pilot line design based on 18650 battery testing	85 days	Mon 1/2/23	Fri 4/28/23	28,32
30		Pilot line for scaled-up material production established	0 days	Fri 4/28/23	Fri 4/28/23	29
31	**6.0**	**Production of Industrial Battery Prototypes**	**170 days**	**Mon 8/1/22**	**Fri 3/24/23**	
32		Produce and test initial 18650 batteries	110 days	Mon 8/1/22	Fri 12/30/22	19
33		Initial set of industry-standard batteries produced	0 days	Fri 12/30/22	Fri 12/30/22	32
34		Refine further prototypes for production	60 days	Mon 1/2/23	Fri 3/24/23	32



Schedule Summary

Task	Description	Year 1				Year 2				Year 3			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1.0	Project Management & Planning												
2.0	Formulation and Production of Test Samples												
M1	Capabilities to Test Powders Established												
3.0	In-House Materials Testing												
4.0	Selection of Best SiOC and Coal Formulations												
M2	Best Coal Material Identified												
M3	Best Overall Composition Identified												
M4	Production and Testing Capability for Pouch Cells Identified												
5.0	Scale Up Production												
M6	Pilot line for scaled-up material production established												
6.0	Production of Industrial Battery Prototypes												
M5	Initial set of industrial standard batteries produced												