

## CLEAN RESOURCES FINAL REPORT PACKAGE

Project proponents are required to submit a Final Report Package, consisting of a Final Public Report and a Final Financial Report. These reports are to be provided under separate cover at the conclusion of projects for review and approval by Alberta Innovates (AI) Clean Resources Division. Proponents will use the two templates that follow to report key results and outcomes achieved during the project and financial details. The information requested in the templates should be considered the minimum necessary to meet AI reporting requirements; proponents are highly encouraged to include other information that may provide additional value, including more detailed appendices. Proponents must work with the AI Project Advisor during preparation of the Final Report Package to ensure submissions are of the highest possible quality and thus reduce the time and effort necessary to address issues that may emerge through the review and approval process.

### *Final Public Report*

The Final Public Report shall outline what the project achieved and provide conclusions and recommendations for further research inquiry or technology development, together with an overview of the performance of the project in terms of process, output, outcomes and impact measures. The report must delineate all project knowledge and/or technology developed and must be in sufficient detail to permit readers to use or adapt the results for research and analysis purposes and to understand how conclusions were arrived at. It is incumbent upon the proponent to ensure that the Final Public Report **is free of any confidential information or intellectual property requiring protection**. The Final Public Report will be released by Alberta Innovates after the confidentiality period has expired as described in the Investment Agreement.

### *Final Financial Report*

The Final Financial Report shall provide complete and accurate accounting of all project expenditures and contributions over the life of the project pertaining to Alberta Innovates, the proponent, and any project partners. The Final Financial Report will not be publicly released.

*Alberta Innovates is governed by FOIP. This means Alberta Innovates can be compelled to disclose the information received under this Application, or other information delivered to Alberta Innovates in relation to a Project, when an access request is made by anyone in the general public.*

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## CLEAN RESOURCES FINAL PUBLIC REPORT TEMPLATE

### 1. PROJECT INFORMATION:

<b>Project Title:</b>	<b>Machine Learning-Assisted Electrolyte Optimization for Next Generation</b>
<b>Alberta Innovates Project Number:</b>	212201721
<b>Submission Date:</b>	September 15, 2023
<b>Total Project Cost:</b>	\$530,445 CAD
<b>Alberta Innovates Funding:</b>	\$221,000 CAD
<b>AI Project Advisor:</b>	Susan Carlisle

### 2. APPLICANT INFORMATION:

<b>Applicant (Organization):</b>	<b>Nanode Battery Technologies Ltd.</b>
<b>Address:</b>	9214 116 ST NW, Edmonton, AB T6G1R1
<b>Applicant Representative Name:</b>	Bing Cao
<b>Title:</b>	CEO
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### 3. PROJECT PARTNERS

Please provide an acknowledgement statement for project partners, if appropriate.

*RESPOND BELOW*

We thank the University of Alberta, the National Research Council of Canada's Industrial Research Assistance Program (IRAP), Levven, GreenSTEM, and VDL group for their contributions and financial contribution to this project.

#### A.

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### EXECUTIVE SUMMARY

Provide a high-level description of the project, including the objective, key results, learnings, outcomes and benefits.

*RESPOND BELOW*

Nanode Battery Technologies uses machine learning (ML) based approaches to optimize electrolyte and novel anode materials compatibility, thus increasing the capacity and cycle life of Lithium-ion batteries (LIBs) anodes. Nowadays, novel anode materials are innovated to improve the performance of LIBs. Alternative electrolytes also need to be designed in tandem with anodes to further improve battery properties. Currently, electrolyte composition is empirically screened. There are over 10100 possibilities to synthesize active materials and prepare electrolytes. Nanode applies Design of Experiments (DOE) and ML approaches to generate a dataset and build an integrated platform for electrolyte optimization and battery life improvement.

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### B. INTRODUCTION

Please provide a narrative introducing the project using the following sub-headings.

- **Sector introduction:** Include a high-level discussion of the sector or area that the project contributes to and provide any relevant background information or context for the project.
- **Knowledge or Technology Gaps:** Explain the knowledge or technology gap that is being addressed along with the context and scope of the technical problem.

*RESPOND BELOW*

#### **Sector introduction**

Our primary target market is battery startups and original equipment manufacturers (OEMs) who want to take advantage of Nanode's cost-effective anode to improve the performance of their products and accelerate market entry. We also look forward to helping startups and battery OEMs, specifically

those developing novel battery components, to reduce their R&D cost and shorten the time to market using our experience and methods in the data-driven optimization pipeline we used during this project.

### Knowledge or Technology Gaps

While tin has the potential to increase the energy density of battery packs for electric mobility applications, it has low initial coulombic efficiency and low cycle life. One possibility to improve these parameters is by changing the composition of electrolytes. However, there are several solvents and salts to be considered and, for each combination, the relative contents of the components also need to be explored to find the optimum combination. This complexity spans more than tens of billions of candidate electrolyte formulations, hence the traditional experimentation is not suitable for this optimization. Therefore, we turned to machine learning to optimize the electrolyte formulation.

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## C. PROJECT DESCRIPTION

Please provide a narrative describing the project using the following sub-headings.

- **Knowledge or Technology Description:** Include a discussion of the project objectives.
- **Updates to Project Objectives:** Describe any changes that have occurred compared to the original objectives of the project.
- **Performance Metrics:** Discuss the project specific metrics that will be used to measure the success of the project.

*RESPOND BELOW*

### Knowledge or Technology Description

The main objectives of this project are given below.

- (1) Build machine learning pipelines to use electrolyte data and cell data for the optimization of initial coulombic efficiency and cycle life.
- (2) Improve the initial coulombic efficiency to 85 %.
- (3) Improve the cycle life to 500 cycles (target revised to 300 cycles during the project).

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## D. METHODOLOGY

Please provide a narrative describing the methodology and facilities that were used to execute and complete the project. Use subheadings as appropriate.

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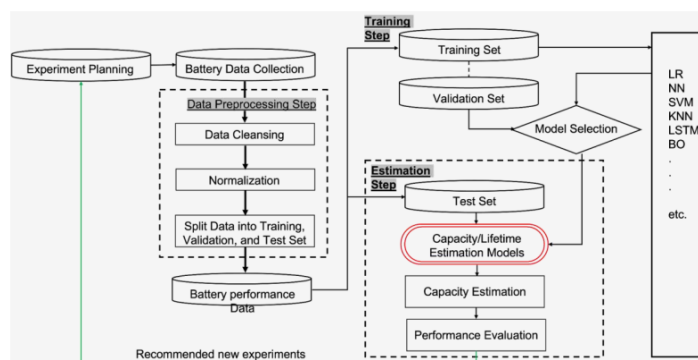


Figure1. Schematic representation of machine learning assisted closed-loop optimization platform.

### Feasibility Study and Preliminary Model Testing Using Thin Film Data (Milestones 1 and 2)

Our goal was to improve the two key performance indicators (initial coulombic efficiency and cycle life) of Li-ion cells for our ribbon anodes using machine learning-based experiments. We initially used Sn thin film (100 nm deposited on a stainless-steel substrate) and collected the initial coulombic efficiency and capacity retention at cycle 50 (as an indicator of cycle life). Capacity retention at cycle 50 (R50) was used as a proxy for cycle life for two reasons (i) it takes 6-10 weeks to acquire cycle life for each cell, and (ii) the number of experiments we could run parallelly was limited by our instrumental capacity. Using the thin film data, we tested several machine learning approaches such as linear regression, random forest regression, gradient boosting trees regression, and Bayesian optimization. The project scheme is described in Figure 1.

### Experimental Planning and Cell Testing (Milestone 3)

We tested more than 200 cells with ribbon anodes and around 150 cells with thin film anodes in this project. Across ribbons and thin films, more than 90 electrolytes were tested, including compositions from Bayesian optimization iterations.

### Optimization of Initial Coulombic Efficiency (Milestones 4, 5, and 6)

From the preliminary model testing results using thin film data, we selected the best approach and first tested it for the optimization of the initial coulombic efficiency for our ribbons.

### Optimization of Cycle Life (Milestones 4, 5, and 6)

For the cycle life optimization, since it takes a long time to acquire the cycle life data, we focused on (i) analyzing the existing data to find and exploit trends to improve cycle life and (ii) using machine learning to predict cycle life using early cycling data (i.e., predict cycle life from 10 days of cycling data). We then used the cycle life prediction model and the best machine learning approach to optimize the cycle life.

### Web Based Platform for Data Storage, Visualization, and Machine Learning (Milestone 6)

In order to track the cell data and integrate machine learning models, such as the cycle life prediction model, we revamped our old data tracking system. The new additions to this platform include the Neware data viewer and the cycle life prediction model.

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## E. PROJECT RESULTS

Please provide a narrative describing the key results using the project's milestones as sub-headings.

- Describe the importance of the key results.
- Include a discussion of the project specific metrics and variances between expected and actual performance.

RESPOND BELOW

### Feasibility Study and Preliminary Model Testing Using Thin Film Data (Milestones 1 and 2)

The feasibility study was performed by Alberta Machine Intelligence Institute (AMII), which concluded that machine learning would be a viable solution for our optimization problem. AMII recommended testing several models, such as decision tree, gradient boosting trees, and Gaussian processes using open-source implementation available from Scikit-Learn<sup>1</sup> library, and then adoption of the best method for experimental optimization. Based on their recommendation and literature on machine learning studies in chemistry, we tested linear regression, symbolic regression, ada boost regression, random forest regression, gradient boosting trees regression, and Gaussian processes (with Bayesian optimization) for initial coulombic efficiency and capacity retention at cycle 50.

### Experimental Planning and Cell Testing (Milestone 3)

Due to the time constraint caused by the personnel change, this work was carried out in parallel with milestones 4-6. More than 200 cells with ribbon anodes were tested for initial data collection based on predictions from data analysis and machine learning.

### Optimization of Initial Coulombic Efficiency (Milestones 4, 5, and 6)

Based on the outcome of the feasibility study, we used the Bayesian optimization (BO) method to improve the initial coulombic efficiency (ICE). We started this optimization using samples with  $\leq 70\%$  ICE and then, by closely following the BO performance on the feasibility study and the experiments, we identified that an additional delithiation step can improve the ICE and used it to improve the ICE to 85 %.

### Optimization of Cycle Life (Milestones 4, 5, and 6)

For this task, we built a model to predict cycle life using the data from the first 30 cycles. For the cycle life improvement, based on exploration of our limited data on ribbon anodes, we identified a relationship between the cycle life and the specific capacity of the ribbon anode. We carried out further experimentation to validate this observation. Validation of the cycle life/specific capacity relationship enabled us to understand the failure mechanism of our anode and directed us to investigate the structure and composition of the anode for further optimization of cycle life. Using this method, we validated our

assumption and carried out new experiments, by which we increased the cycle life of our ribbon anode from 325 to 407.

#### **Web Based Platform for Data Storage, Visualization, and Machine Learning (Milestone 6)**

We created a new web-based application for tracking results from battery cycling experiments. This new application was created to enable the easier incorporation of machine learning models in the future for better experimental designs. We have added the capability to track and visualize results from our new Neware battery testing system with 344 channels. In addition, we have added the cycle life prediction model to this web application.

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## **F. KEY LEARNINGS**

**Please provide a narrative that discusses the key learnings from the project.**

- Describe the project learnings and importance of those learnings within the project scope. Use milestones as headings, if appropriate.
- Discuss the broader impacts of the learnings to the industry and beyond; this may include changes to regulations, policies, and approval and permitting processes

*RESPOND BELOW*

#### **Feasibility Study and Preliminary Model Testing Using Thin Film Data (Milestones 1 and 2)**

Our feasibility studies on the thin film data showed that ICE was predicted with a much lower error rate (5.0 %) compared to R50 (13.4 %) by the random forest regression model. The error for linear regression and ada boost regression was higher. In the case of gradient boosting regression, although the prediction error for R50 is slightly better than that of random forest (13.4 % vs 13.8 %), we selected random forest as the best since the difference between train and test error was lower for random forest. In addition to these models, we also tested Gaussian process with Bayesian optimization (BO) approach for both ICE, R50 independently

and for a combined objective ( $\frac{1}{2}\text{ICE} + \frac{1}{2}\text{R50}$ ). BO tests were started with 5 initial data with low values

( $\leq 60$  % for both ICE and R50) and BO guided experiments reached more than 20 % improvement within 20 experiments. The results are given in Figure 2. Based on these tests, we selected Bayesian optimization for the optimization of ICE and the cycle life of our ribbon anodes.

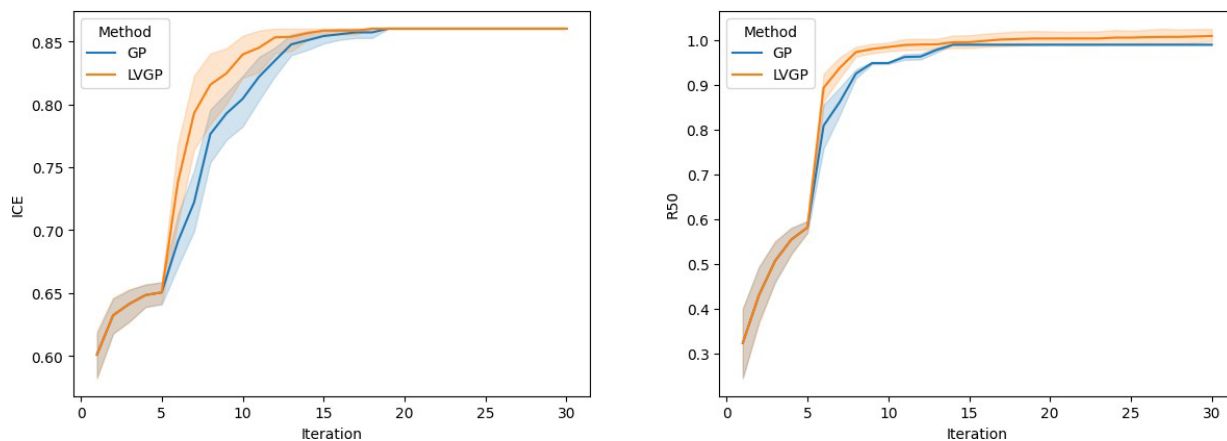


Figure 2. Bayesian Optimization of ICE (left) and R50 (right) using Gaussian process (GP) and latent-variable Gaussian process (LVGP). The results show the average performance of 30 runs.

### Optimization of Initial Coulombic Efficiency (Milestones 4, 5, and 6)

Based on the BO simulation results using the thin film data, we began the ICE optimization of our ribbon anodes with a fixed composition and fabrication method. We started with 5 data points from the existing ribbon data. Next, at each cycle, the Gaussian process model was used to predict the ICE for candidates in the selected search space. Then the expected improvement acquisition function was used to select the next sample for experimental evaluation. Cells with the selected electrolyte composition were made and the ICE was measured experimentally. The result was added to the dataset and the model was retrained for the next iteration and repeated for 13 iterations. We found that the ICE of the ribbon showed a slight improvement of 1.5 % from the baseline (70 %), which shows significant underperformance compared to the BO runs on the thin film data (Figure 2). At this point, we looked into the difference between the thin-film and ribbon, and the experimental parameters. Recent literature on tin sheet anodes shows that the state of charge of tin anodes has a significant impact on the ICE.<sup>2</sup> This is a result of the difference in Li-ion diffusivities among the different Li-Sn alloys formed during lithiation. The diffusivity of  $Li_xSn$  alloys with  $x \leq 1$  is lower by an order of magnitude compared to the diffusivity of Li in phases with  $x > 1$ . For the thin film samples, we charged them to full capacity, whereas the ribbon anodes were charged between 10 – 15 % of the theoretical capacity of tin. At 10-15 % of the capacity, the Li-Sn phases formed are in the low diffusivity region. Hence, the diffusivity of the Li may be the main bottleneck. To validate this, we started cells with our baseline electrolyte and at the end of delithiation at the control rate (C/10), it achieved an ICE of 70 %, as expected. Then, we added a second delithiation step with a much lower delithiation rate (C/100) and this resulted in an extra 15 %, bringing the ICE to 85 % (Figure 3). Further improvement can be obtained by increasing the state of charge.



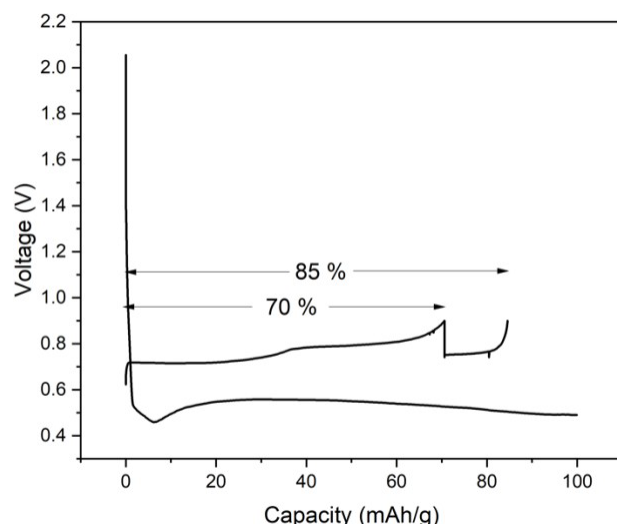


Figure 3. Capacity-potential (vs  $\text{Li}^+/\text{Li}$ ) curve showing the increase in the initial coulombic efficiency upon adding a second delithiation (C/100) following the delithiation at C/10.

### Optimization of Cycle Life (Milestones 4, 5, and 6)

For this task, we developed a model to predict cycle life from early cycling data. We also analyzed the data from cells with ribbon anodes to identify trends.

### Cycle Life Prediction (Milestones 4, 5, and 6)

Studies have shown that the cycle life of Li-ion batteries can be predicted using early cycling data. For example, variation in the discharge capacity vs. voltage curves between cycles 10 and 100 can be used to predict the cycle life of Li-ion batteries with a Mean Absolute Percentage Error (MAPE) of 9.1 %.<sup>3</sup> Other features from the cycling data, such as the difference between the end of charging and discharging potentials, and changes in the differential capacity – differential potentials, can also be used to predict the cycle life of Li-ion batteries with graphite anodes.<sup>4,5</sup> Since no such models were reported for cells with tin anodes, we built a model to predict cycle life for our cells. The model uses the difference in charging curves from cycles 10 and 30 as the feature and is able to predict the logarithm of the cycle life with a MAPE of 2.8 % and a Pearson's correlation coefficient of 0.8.

### Cycle Life Optimization (Milestones 4, 5, and 6)

During the initial data analysis of thin film cells and ribbon cells, we identified a correlation between mass and cycle life. To verify this relationship, we started with ribbons that have varying masses while using the baseline electrolyte to remove any effects of electrolyte on the cycle life. The results are given in Figure 4. It shows that for a given specific capacity, cycle life can vary by more than 100 cycles. However, the standard

deviation of cycle life for samples within a 5 mAh/g window is around 50 cycles. We attribute this deviation to the experimental changes during the manufacturing of ribbons and the cell assembly. For analysis, we focused on the maximum cycle life for a given capacity range due to the size of the dataset. Another observation from Figure 4 is that despite the electrolyte composition, the variation in the maximum cycle life can be explained by the change in the specific capacity. To validate this, we tested cells with a specific capacity of 50 mAh/g and then measured their cycle life. The predicted cycle life for this capacity is 400 cycles and the experimentally obtained values are 396, 399, 404, and 407. The reproducible agreement of experimental cycle life with the predicted value confirms the dependence between the specific capacity and cycle life and opens a question on the mechanism.

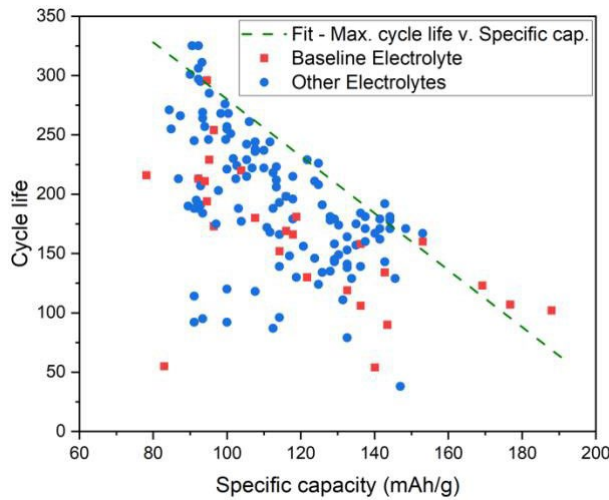


Figure 4. Specific capacity vs cycle life of cells with ribbon anodes and with different electrolytes. Baseline electrolyte is represented in red squares while other electrolytes are represented collectively in blue circles.

During the development of the cycle life prediction model, we found that the capacity due to Li-Sn phases up to  $x = 1$  increases with cycling initially and then the increase slows down before decreasing rapidly (Figure 5). The rapid decrease coincides with the cell failure. Moreover, the difference between this capacity at cycle 10 and 30 increases with cycle life. Studies on tin anodes have shown that although the tin expands upon lithiation, it does not reduce to its original volume upon delithiation and forms a porous structure instead.<sup>6-8</sup> Based on this report and our analysis of cycling data, we hypothesize that the increased porosity leads to the increase in the formation of lower lithiated phases ( $Li_xSn, x \leq 1$ ) compared to the previous cycle. This increases the porosity of the anode with cycling and the increasingly porous structure undergoes mechanical failure to form smaller particles at the expense of the monolithic ribbon. Since there are no binder and conductive agents present to physically and electrically bind the particles, the cell fails at this stage.

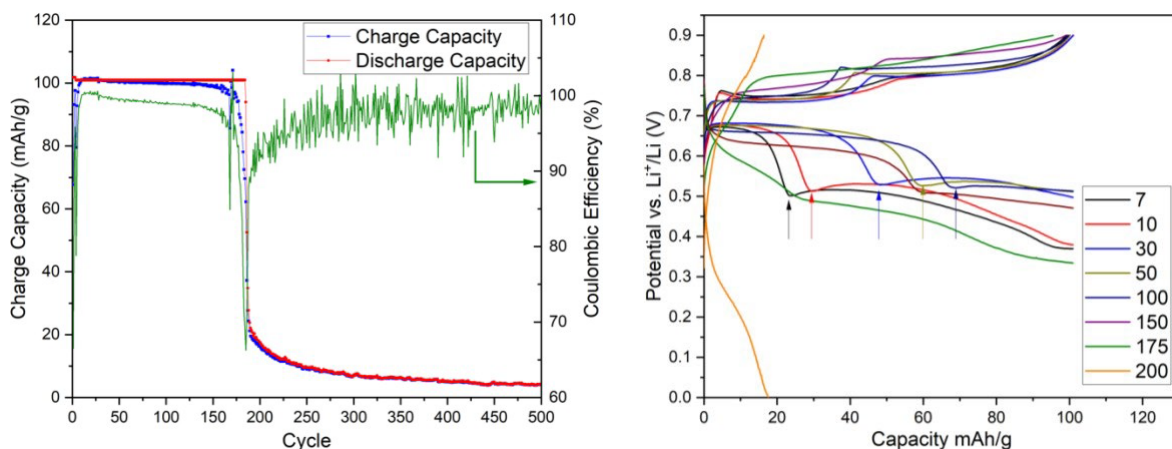


Figure 5. Cycle vs specific capacity (left) and specific capacity vs potential at different cycles (right). The vertical arrows in the right plot show the end of the formation of  $\text{LiSn}$ .

## References

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## G. OUTCOMES AND IMPACTS

Please provide a narrative outlining the project's outcomes. Please use sub-headings as appropriate.

- **Project Outcomes and Impacts:** Describe how the outcomes of the project have impacted the technology or knowledge gap identified.
- **Clean Energy Metrics:** Describe how the project outcomes impact the Clean Energy Metrics as described in the *Work Plan, Budget and Metrics* workbook. Discuss any changes or updates to these metrics and the driving forces behind the change. Include any mitigation strategies that might be needed if the changes result in negative impacts.
- **Program Specific Metrics:** Describe how the project outcomes impact the Program Metrics as described in the *Work Plan, Budget and Metrics* workbook. Discuss any changes or updates to these metrics and the driving forces behind the change. Include any mitigation strategies that might be needed if the changes result in negative impacts.
- **Project Outputs:** List of all obtained patents, published books, journal articles, conference presentations, student theses, etc., based on work conducted during the project. As appropriate, include attachments.

RESPOND BELOW

### Outcomes and Impacts

The main outcome of this project confirmed that data analysis and machine learning have the potential to accelerate the optimization of battery components. However, the material and electrochemical aspects should be taken into consideration when designing experiments, analyzing the results, and for machine learning. For tin anodes, the diffusivity of Li in different Li-Sn phases has a

significant impact on the initial coulombic efficiency. Improving the cycle life requires the optimization of the anode composition in addition to the electrolyte optimization.

## Clean Energy Metrics

Our initial goals for this project were to (i) increase the cycle life to 500 and (ii) increase the initial coulombic efficiency to 85 %. Due to the delay caused by the personnel change, we revised the cycle life goal to 300. Using data-based approaches, we have achieved a cycle life of 407 and an initial coulombic efficiency of 85 %.

## Clean Resources Metrics

Metric	Project Target	Commercialization / Mobilization	Comments (as needed)
Investment in 4 Core Strategic Technology Areas	\$508,615	\$500K	Achieved: This project is associated with Data-Enabled Innovation and Clean Technology. We advanced adoption of machine learning in accelerating the R&D of battery electrolyte optimization. During the project Nanode has raised \$500K from venture capitalists, very close to the Project target.
Jobs: Actual new jobs created from project	2		Achieved: 2 jobs were created at the project start, adding a battery engineer and a machine learning engineer to the Nanode team.
Jobs: Projected new jobs created from future deployment		10+	In five years, the success of this project is expected to create 10+ new positions and train high quality employees with interdisciplinary skills in clean technology, battery, machine learning, and renewable energy.
TRL advancement	Improve from TRL 3 to 7	9	Achieved: Advancement to TRL 7 was achieved.
GHG emissions: Projected reductions from future deployment (to 2030)		2,198,434 tonnes/year	Since we are still in the lab scale production during the project, the GHG emission is negligible. During the project, we have advanced the potential for market adoption of Nanode's anode technologies. Eventually, our technology is expected to make electric vehicles more accessible by making energy storage more efficient. The calculated annual GHG emission reductions from new anodes used for improved battery energy storage at a commercial rollout are forecast to be 114,687 tonnes/year in total once in mass production and 2,198,434 tonnes/year in Canada starting in 2027 when our technology is adopted for electric vehicles and energy storage.
Collaborators	2	5	Exceeded: We established 3 new customers during this project and attracted 5 more customers in our pipeline for material test.
Future Capital Investment		\$12.5M	In the next 6 months, we will raise another \$500k in equity investment for scale up production. In the next two years, we plan to raise \$2.5M in seed investment and \$10M in series A financing.
Sector HQP Trained	5	10	Achieved: Since hiring the machine learning scientist, company staff have been attending monthly machine learning workshops. By 2027, the success of this project is expected to create 10+ new positions and train high quality employees with interdisciplinary skills in clean technology, battery, machine learning, and renewable energy.

## Program Specific Metrics

The feasibility study and the preliminary machine learning tests showed the possibility of using machine learning for the optimization of cycle life and initial coulombic efficiency. With this opportunity in mind, we collected data on more than 200 cells with several electrolytes, and built machine-learning pipelines to import data, analyze, fit models, and make predictions. Based on the results, we used machine learning-based closed-loop optimization to improve the initial coulombic efficiency. Based on the progress of closed-loop optimization and domain knowledge, we improved the initial coulombic efficiency from 70 % to 85 %. By analyzing the data, we increased the cycle life from 325 to 407, a 25 % improvement.

### Program Specific Metrics

GHG emissions: Actual	Project Target	Commercialization / Mobilization	Comments (as needed)
# of renewable energy technologies deployed	1	1	Achieved: Nanode advanced its tin-based anodes to be deployed in lithium and sodium ion batteries.
Clean tech companies with HQ in AB	1	1	Sustained: Nanode is located in Edmonton and will keep headquarter in Edmonton.

### Project Outputs

As of now, we do not have any publication of the results from this project. Our company has benefited significantly from this project. With the updated cycle life and material performance matrix, we were able to attract more customer attention: for lithium ion battery anodes, we successfully passed phase one and phase two tests with one of our customer, a battery manufacturer in the US, and they signed a letter of intent for future purchase; For sodium ion battery anodes, we have initiated two proof of concept projects with two OEM companies and shipped sample anode to them. Beyond the project, we will continue adopting and improving this new digital/machine learning platform we've created to accelerate our R&D process.

### Project Success Metrics

Metric	Project Target	Commercialization / Mobilization Target	Comments (as needed)
Battery cycle life	500	1000	Partially Achieved/Exceeded: An improved battery cycle life from 100 to 407 cycles for existing novel anode material was achieved in lithium ion batteries, which is slightly below the target. We also improved the cycle life of this novel anode material in sodium ion batteries to over 3000 cycle, greatly exceeding the project target.
Reduce number of experiments	20%	50%	Achieved/Exceeded: At the end of the project, we reduced the number of experiments to 20 experiments per 10 cycles improvement for lithium ion batteries, achieving the targeted 20% improvement, and 20 experiments per 500 cycles improvement for sodium ion batteries, a 250% improvement, greatly exceeding the project target.
Number of data processing platform	1		Achieved: A data management system was developed for data processing, visualization, and model fitting.
Number of machine learning model	1		Achieved: A closed-loop ML system connecting input and output parameters to guide electrolyte was developed.

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## H. BENEFITS

Please provide a narrative outline the project's benefits. Please use the subheadings of Economic, Environmental, Social and Building Innovation Capacity.

- **Economic:** Describe the project's economic benefits such as job creation, sales, improved efficiencies, development of new commercial opportunities or economic sectors, attraction of new investment, and increased exports.
- **Environmental:** Describe the project's contribution to reducing GHG emissions (direct or indirect) and improving environmental systems (atmospheric, terrestrial, aquatic, biotic, etc.) compared to the industry benchmark. Discuss benefits, impacts and/or trade-offs.
- **Social:** Describe the project's social benefits such as augmentation of recreational value, safeguarded investments, strengthened stakeholder involvement, and entrepreneurship opportunities of value for the province.
- **Building Innovation Capacity:** Describe the project's contribution to the training of highly qualified and skilled personnel (HQSP) in Alberta, their retention, and the attraction of HQSP from outside the province. Discuss the research infrastructure used or developed to complete the project.

*RESPOND BELOW*

### Economic

The potential benefits of this project revolve around electric mobility and the growth of Nanode Battery Technologies Inc. to a revenue generating commercial enterprise. Our products aim to increase the energy density of batteries for electric vehicles while reducing the cost of manufacturing. In addition, machine learning based accelerated battery optimization services create new opportunities in research, development and manufacturing of batteries, as well as providing a service to help grow battery startups and attract new investment to Alberta.

### Environmental

Our products benefit the environment primarily by helping to reduce the emission of greenhouse gases. Since the main market for our products is electric mobility, the increase in the adoption of electric vehicles will contribute to the reduction of tailpipe emissions.

### Social

The social benefits include the encouragement of new startups in the transition to a low emissions economy and society. Our services can help to build the startup culture, support PSI research and development and lead to new jobs for highly skilled personnel in Alberta's emerging battery value chain.

## Building Innovation Capacity

Commercialization of our products will create more training and development to existing and new HQSP in Alberta.

I.

### RECOMMENDATIONS AND NEXT STEPS

Please provide a narrative outlining the next steps and recommendations for further development of the technology developed or knowledge generated from this project. If appropriate, include a description of potential follow-up projects. Please consider the following in the narrative:

- Describe the long-term plan for commercialization of the technology developed or implementation of the knowledge generated.
- Based on the project learnings, describe the related actions to be undertaken over the next two years to continue advancing the innovation.
- Describe the potential partnerships being developed to advance the development and learnings from this project.

RESPOND BELOW

In this project, we have identified that by using domain knowledge, data analysis, and machine learning battery properties can be improved. However, continuous efforts are needed to further refine the ML models and improve the cycling performance, in order to commercialize our anodes for the Li-ion battery market. Meanwhile, our sodium-ion batteries have reached cycle life of over 1000 for ribbons and more than 5000 for powders in extremely fast charging conditions. Hence in the short term, we dedicate our efforts to optimizing the electrolyte for sodium-ion batteries according to our customer needs using machine learning and domain knowledge. At the same time, we will continue optimizing the structure, composition, and electrolyte of our anodes for Li-ion batteries.

J.

### KNOWLEDGE DISSEMINATION

Please provide a narrative outlining how the knowledge gained from the project was or will be disseminated and the impact it may have on the industry.

RESPOND BELOW

As of now, we do not have any publication of the results from this project.

We have created an online ML platform for battery cycle life optimization, which can be adopted in the industry for materials, e.g., the cathode or electrolyte, discovery and optimization. We also have proved that ML is an efficient way to reduce the R&D time. By adopting this method, we have delivered two battery anodes to the lithium and sodium ion battery market.



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## K. CONCLUSIONS

**Please provide a narrative outlining the project conclusions.**

- Ensure this summarizes the project objective, key components, results, learnings, outcomes, benefits and next steps.

*RESPOND BELOW*

We started this project to improve the cycle life and initial coulombic efficiency of our ribbon anodes for Li-ion batteries using machine learning methods. During this project, we have conducted more than 200 cell experiments, built pipeline to analyze and fit machine learning models. Using domain knowledge, data analysis, and machine learning methods, we improved the cycle life by 25 % and the initial coulombic efficiency by 15 % from the baseline. In the future we will continue to use the knowledge gained in using machine learning in order to reach commercial targets. In addition, we will also use the knowledge and experience to optimize electrolytes for sodium ion batteries according to our customer needs.