Program Profile		
Program	Program name	"Computational analysis of electrochemical behaviors of commercial lithium-ion batteries on various thermal conditions."
	Category	A1

Summary of Program	
Program Name	"Computational analysis of electrochemical behaviors of commercial lithium-ion batteries on various thermal conditions."
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Abstract of Program	The performance, safety, and lifespan of lithium-ion batteries are significantly influenced by thermal conditions, which directly affect their electrochemical behavior. This project aims to conduct a comprehensive computational analysis of commercial lithium-ion batteries under varying thermal environments to understand the coupled thermal-electrochemical dynamics. Multiphysics simulations will be carried out using ANSYS and COMSOL Multiphysics to model heat generation, ion transport, and potential distribution within the cell architecture. MATLAB and Python will be employed for parametric data analysis, result visualization, and comparative evaluation. The computational models will be validated using open-source experimental datasets to ensure accuracy and reliability. The study intends to provide valuable insights into battery performance and thermal stability, aiding in the design of safer and more efficient battery systems for real-world applications.

Details of Program		
Planning		
Objectives	Long-term Goals	• Develop a validated multiphysics framework for analyzing the coupled thermal–electrochemical behavior of commercial lithium-ion batteries. • Support the design of safer, more efficient, and longer-lasting batteries for applications in electric vehicles, renewable energy storage, and portable electronics. • Contribute to national and global efforts in clean energy transition, climate resilience, and sustainable energy technologies. • Establish the World University of Bangladesh as a research hub in simulation-driven battery engineering and energy storage innovation.
	Short-term Targets	• Complete multiphysics simulation models in COMSOL and ANSYS for baseline thermal and electrochemical performance. • Validate computational results with open-source experimental datasets to ensure accuracy and reproducibility. • Develop data analysis scripts in MATLAB and Python for automated result processing and visualization. • Publish at least two Scopus-indexed journal/conference papers by the end of the project timeline. • Train student researchers in computational modeling, thermal management, and data-driven analysis.

<table>
<tr><td></td><td>Rationale</td><td>Bangladesh faces urgent challenges in urban mobility, environmental sustainability, and road safety. The Effi-Que ADAS EV project responds to these issues by empowering students to design and build a smart electric vehicle equipped with Advanced Driver Assistance Systems (ADAS). It aligns with national priorities for clean mobility and prepares students for industry through hands-on experience in engineering, fabrication, and innovation. The initiative bridges academic learning with real-world application, fostering interdisciplinary collaboration and positioning WUB as a leader in sustainable transport education.</td></tr>
<tr><td rowspan="2">Subject (Leader)</td><td>Initiator(s)</td><td>Ahmad Abdullah Mujahid</td></tr>
<tr><td>Champion(s)</td><td>Ahmad Abdullah Mujahid</td></tr>
<tr><td rowspan="3">Environment</td><td>Nature/Society</td><td>This research contributes to environmental sustainability by improving the thermal safety and performance of lithium-ion batteries, which are critical for clean energy applications like electric vehicles and renewable energy storage. Safer and longer-lasting batteries support a transition to low-carbon societies.</td></tr>
<tr><td>Industry/Market</td><td>The findings can help battery manufacturers and electric vehicle producers optimize battery designs for better thermal management. Improved modeling tools may also accelerate product development cycles and reduce reliance on physical prototypes.</td></tr>
<tr><td>Citizen/Government</td><td>The project aligns with national and international goals for energy efficiency, green mobility, and climate change mitigation. The research can support policy decisions regarding battery safety standards, thermal testing protocols, and electric mobility incentives.</td></tr>
<tr><td rowspan="3">Resources</td><td>Human resources</td><td>The project requires researchers with expertise in electrochemistry, thermal-fluid sciences, and computational modeling. Additional support may come from data analysts familiar with Python and MATLAB.</td></tr>
<tr><td>Financial resources</td><td>Funding is needed for software licenses (COMSOL, ANSYS, MATLAB), computing infrastructure, publication fees, and possibly conference travel for dissemination.</td></tr>
<tr><td>Technological resources</td><td>High-performance computing facilities for simulation, access to open-source battery datasets, and integration platforms for data processing and visualization (e.g., Python libraries, MATLAB toolboxes).</td></tr>
<tr><td>Mechanism</td><td>Strategy (Weight/Sequence)</td><td>High Weight / Early Execution:
• Development of baseline electrochemical and thermal models.
• Validation of computational results using open-source experimental data.

Medium Weight / Parallel Execution:
• Integration of simulation workflows (COMSOL, ANSYS, MATLAB, Python) for efficiency.
• Sensitivity and parametric studies to quantify thermal effects on performance.

Lower Weight / Later Execution:</td></tr>
</table>

		• Dissemination of findings through publications, conferences, and curriculum integration. • Application of models for optimization, control strategies, and industry collaboration.
	Organization	• Core Research Team: Led by the principal investigator with expertise in electrochemistry and computational modeling. • Supporting Roles: Student researchers for simulation and data analysis; technical staff for computing infrastructure. • External Input: Guidance from industry stakeholders and open-source user communities for model relevance and troubleshooting. • Responsible Institution: World University of Bangladesh, with academic oversight and administrative support for project execution.
	Culture	• Collaborative: Encourages interdisciplinary work across mechanical, electrical, and computer science departments. • Innovation-Oriented: Promotes the adoption of advanced simulation technologies as alternatives to costly experimental testing. • Transparent and Reproducible: Ensures credibility through open validation datasets and standardized workflows. • Capacity-Building: Fosters student training, skill development, and curriculum enrichment in energy storage and computational engineering.
Doing		
Launch date		July 2025
Responsible organization		World University of Bangladesh
Program content and process		This program focuses on the computational investigation of electrochemical and thermal behaviors of commercial lithium-ion batteries under diverse temperature conditions. The process begins with a literature review to establish baseline knowledge, followed by the development of physics-based electrochemical models. These models are coupled with thermal simulations using COMSOL Multiphysics and ANSYS to capture heat generation, ion transport, and potential distributions. MATLAB and Python are employed for parametric studies, sensitivity analysis, and visualization. Validation is conducted against open-source experimental datasets to ensure accuracy. The program concludes with the preparation of scientific publications, dissemination through conferences, and integration into academic teaching modules.
Key highlights of the content/process		• Interdisciplinary Integration: Combines electrochemistry, thermal sciences, and computational modeling.

	• Advanced Simulation Tools: Employs COMSOL, ANSYS, MATLAB, and Python for a complete modeling workflow. • Validation and Transparency: Results are benchmarked against publicly available datasets, ensuring credibility. • Practical Relevance: Addresses critical challenges in battery safety, efficiency, and thermal management for EVs, renewable energy storage, and portable electronics. • Capacity Development: Provides training opportunities for students and contributes to research-driven curriculum development.
Differences from traditional approaches	• Reduced Reliance on Physical Testing: Unlike conventional studies that depend on laboratory experiments, this project uses computational models to minimize cost and time. • Enhanced Insights: Provides internal battery parameters (temperature gradients, state-of-charge distribution) that are difficult to measure experimentally. • Scalability and Flexibility: Models can be adapted to different cell geometries, chemistries, and operating conditions. • Automated Analysis: Incorporates scripting tools (Python/MATLAB) for efficient data handling, visualization, and reproducibility. • Transparency: Uses open-source validation datasets, which are often missing in closed laboratory research.
Progress as of today	• Completed comprehensive literature review on thermal-electrochemical behavior of commercial lithium-ion batteries. • Developed initial geometry and physics-based models in COMSOL Multiphysics and ANSYS. • Set up thermal boundary conditions and electrochemical coupling parameters. • Collected and pre-processed open-source experimental datasets for model validation. • Started simulation runs for ambient and elevated temperature cases. • Developed data analysis scripts in Python and MATLAB for result post-processing and visualization.
Problems in implementation	• Complexity in multiphysics coupling: Accurately combining thermal and electrochemical processes in a stable simulation is computationally demanding. • High simulation time: Full-cell simulations at fine mesh resolutions are taking longer than expected. • Data compatibility: Matching available experimental data formats with simulation outputs for validation requires preprocessing. • Software limitations: Licensing restrictions or solver convergence issues (particularly in ANSYS) are occasionally interrupting workflows.

Approaches to solve the problems	• Simplifying models where possible by using symmetry or 2D approximations for faster iteration and debugging. • Using batch processing and mesh optimization to reduce computational load. • Standardizing data formats and creating custom Python scripts to bridge between simulation output and validation datasets. • Consulting software documentation and community forums, and reaching out to university or open-source user communities for solver troubleshooting. • Considering parallel simulation strategies on high-performance computing (HPC) resources where available.
Completion date, if completed	• The project is ongoing. • Estimated completion date: October 2025, including final validation, reporting, and documentation.
Seeing	
Impacts on students	• Contributes to the university's research output and reputation in the field of sustainable energy and simulation-based engineering. • Supports professors in research funding applications by showcasing a working, validated computational model. • Creates a foundation for future projects, PhD proposals, and international academic exchange. • Strengthens the university's curriculum in battery technology, energy systems, and computational modeling. • Promotes cross-department collaboration (e.g., mechanical, electrical, and computer science disciplines).
Impacts on professors	• Positive interest from battery manufacturers and electric vehicle companies in validated, predictive modeling tools that can reduce R&D costs. • Recognition of the model's potential to improve battery design and thermal management strategies. • Opens opportunities for industry-academia collaboration on performance testing, model customization, and software integration. • May influence R&D decisions by providing data-driven insights into failure modes and efficiency limits under thermal stress.
Impacts on university administration	• Institutional Reputation: Strengthens the standing of the World University of Bangladesh by positioning it as a pioneer in advanced computational energy research. • Strategic Research Growth: Provides a flagship project that aligns with global sustainability and clean energy agendas, supporting future funding and collaborations. • Policy and Decision Support: Offers validated research outputs that can inform university-level strategies for promoting innovation, interdisciplinary projects, and industrial partnerships. • Capacity Building: Enhances faculty expertise in cutting-edge modeling tools (COMSOL, ANSYS, MATLAB, Python), which can be integrated into curricula and future research.

	• Resource Optimization: Reduces dependency on costly experimental setups by adopting simulation-driven methodologies, helping the university manage financial and laboratory resources more effectively. • International Visibility: Increases opportunities for global collaboration and exchange programs through publications, conferences, and alignment with international research priorities.
Responses from industry/market	• Aligns with national and international goals for clean energy, electric mobility, and climate resilience. • Potential for support or recognition under government-funded energy innovation or digital transformation initiatives. • Provides a validated framework that can be used to inform policy and safety standards for battery usage and thermal testing. • Encourages inclusion in strategic technology roadmaps or energy transition programs.
Responses from citizen/government	N/A
Measurable output (revenues)	Technical outputs: • Validated thermal-electrochemical model • Simulation results across thermal ranges • Analytical scripts and visualizations Academic outputs: • 2/journal/conference publications • Seminar/workshop presentations
Measurable input (expenses)	Measurable Input (Expenses) Software Licenses • COMSOL Multiphysics, ANSYS, MATLAB (academic versions) • Estimated Cost: Medium to High • Justification: Essential for simulation modeling and analysis. Computing Infrastructure • High-performance computing (HPC) access, storage, and backup systems • Estimated Cost: Moderate • Justification: Required for running large-scale multiphysics simulations efficiently. Human Resources • Research assistants, graduate students, and technical staff training • Estimated Cost: Moderate • Justification: Builds long-term institutional capacity and ensures timely project execution. Data Acquisition and Management • Collection, preprocessing, and storage of open-source datasets • Estimated Cost: Low • Justification: Data is freely available, but requires organization and processing. Publication and Dissemination • Journal submission fees, conference registration, and presentation costs

<table>
<tr><td></td><td>Estimated Cost: Low to Moderate
Justification: Necessary for visibility, credibility, and academic impact.
Contingency and Miscellaneous
Minor costs for software troubleshooting, workshops, or collaborations
Estimated Cost: Low
Justification: Provides flexibility to address unforeseen technical or administrative needs.</td></tr>
<tr><td>Cost-benefit analysis for effectiveness</td><td><table>
<tr><th>Item</th><th>Cost/Investment</th><th>Benefits</th></tr>
<tr><td>Software licenses (COMSOL, ANSYS, MATLAB)</td><td>Medium to High</td><td>Enables advanced simulations; reusable for multiple future projects</td></tr>
<tr><td>Researcher time and training</td><td>Moderate</td><td>Skills development, academic publications, long-term institutional capacity</td></tr>
<tr><td>Computing resources</td><td>Moderate</td><td>High-quality, scalable simulations</td></tr>
<tr><td>Validation data (open-source)</td><td>Low (freely available)</td><td>Increases credibility and transparency</td></tr>
<tr><td>Total Estimated Cost</td><td>Medium (within academic project standards)</td><td>High return in terms of knowledge, output, visibility, and future funding</td></tr>
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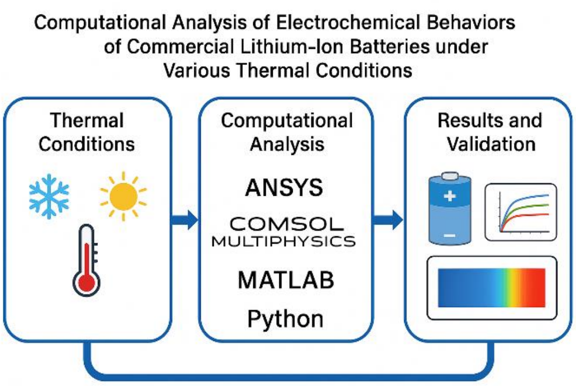
<tr><td colspan="2">Future Planning</td></tr>
<tr><td>Where does the project go from here?</td><td>Model Refinement & Expansion
The next step is to refine the existing thermal-electrochemical models by incorporating more detailed geometry (e.g., 3D full cell) and advanced physics such as aging models, phase change, and SEI formation. This will improve the model’s fidelity and practical relevance.
Simulation of Real-World Load Profiles
Simulations will be extended to include real-world duty cycles, fast charging/discharging conditions, and ambient temperature fluctuations—mirroring conditions in electric vehicles, renewable storage, and consumer electronics.
Degradation and Lifetime Prediction
Incorporate cycle aging and degradation models to predict performance over time. This will help in estimating the usable life and safe operation limits of batteries under different thermal environments.
Experimental Collaboration (Optional but Valuable)</td></tr>
</table>

	• Collaboration with experimental labs or access to in-house testing could validate predictions more rigorously beyond open-source data. Hybrid (sim-experimental) modeling could be explored. • Optimization and Control • Use the validated model to develop optimization algorithms (e.g., for thermal management systems or charge-discharge protocols) or design battery management system (BMS) logic that ensures safe and efficient operation. • Publishing and Dissemination • Prepare and submit the findings to peer-reviewed journals and international conferences. Code and simulation frameworks can also be published as open-source packages or supplementary material. • Application for Funding or Scale-Up • Use the results to apply for larger grants or collaborative projects, possibly involving industrial partners or government agencies focused on clean energy or smart transportation. • Integration into Teaching or Curriculum • Convert parts of the project into lab exercises, simulation modules, or thesis projects for mechanical/electrical engineering students—strengthening the academic program.
Addendum	
Exhibits, pictures, diagrams, etc.	
Reports, mimeos, monographs, books, etc.	It is expected to publish two more Scopus-indexed scientific articles within six months.
Others which may help explain the program (including website links)	A final report will be submitted to the university for record-keeping purposes.