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Ph.D. DISSERTATION DEFENSE

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Date and Time:	Wednesday, August 19, 11 AM -1 PM
Location:	Gateway South 216
Title:	Interpretable Surrogate Modeling and Multi-Objective Optimization of Enhanced Phase Change Material Thermal Management Systems for Lithium-Ion Batteries
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ABSTRACT

Effective thermal management is essential to the safety, performance, and service life of lithium-ion batteries, particularly under the rapid charge-discharge rates encountered in electric-vehicle applications. Phase change materials (PCMs) provide an attractive passive cooling solution because of their high latent heat capacity; however, their inherently low thermal conductivity limits heat dissipation and motivates enhancement strategies such as conductive nanoparticles or embedded metal fins. This research presents a comprehensive methodology that advances passive PCM-based battery thermal management from high-fidelity simulation to interpretable, optimization-ready design tools. The research begins with a critical review of battery thermal management technologies, identifying key gaps in the development and evaluation of PCM-based passive cooling systems. An integrated electrochemical-thermal model is developed by coupling the Newman–Tiedemann–Gu–Kim (NTGK) electrochemical battery formulation with an enthalpy-porosity model for phase change. The model is validated against experimental measurements at 1C, 3C, and 5C discharge rates, achieving a 78% reduction in mean squared error (MSE), a 53% reduction in root mean squared error (RMSE), and a coefficient of determination (R^2) of 0.969. The validated model is subsequently used to investigate 25 nanoparticle-enhanced PCM configurations incorporating copper, aluminum, and hybrid nanoparticle formulations. Copper nanoparticles deliver the greatest thermal improvement, reducing peak cell temperature by up to 17.7 K at 10% loading under 5C discharge, while aluminum nanoparticles achieve up to 14.7 K of cooling with a lower density penalty. A hybrid composition containing 4% Cu and 3% Al retains 91% of the maximum thermal benefit while preserving 35% more latent heat storage capacity than the equivalent copper-only configuration.

To extend beyond the limitations of individual studies, transient thermal responses from validated simulations and independent literature sources are harmonized into an openly available dataset comprising 242 battery-cooling cases and 47,488 transient records spanning both nanoparticle-enhanced and fin-enhanced PCM designs. The dataset employs a unified set of dimensionless features, complete source provenance, and standardized data processing to enable consistent comparison across studies. Leave-one-study-out validation demonstrates that conventional random splits substantially overstate model transferability, highlighting the importance of source-aware evaluation for surrogate-model development.

Building upon this dataset, gene expression programming is employed to develop compact, interpretable closed-form surrogate models for dimensionless cell temperature and PCM liquid fraction for both enhancement strategies. The surrogate models are integrated with a three-objective NSGA-III optimization framework that simultaneously minimizes cell temperature, PCM liquid fraction, and material cost while identifying Pareto-optimal designs. The resulting optimization reveals copper nanoparticle loading and fin ratio as the dominant design variables governing thermal performance and cost, enabling thousands of candidate configurations to be evaluated in the time required for a single computational fluid dynamics simulation. Collectively, the methodologies developed in this dissertation establish a scalable, interpretable, and computationally efficient framework for the design and optimization of next-generation passive battery thermal management systems.