VRIJE UNIVERSITEIT BRUSSEL

The faculty of Engineering of the Vrije Universiteit Brussel invites you to attend the public defense leading to the degree of

DOCTOR OF ENGINEERING SCIENCES

of **Tewelde Hailay Gebregeorgis**

The public defense will take place on **Tuesday 9th June 2026 at 4pm** in room **I.0.01** (Building I, VUB Main Campus)

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UNDERSTANDING AND PREDICTION OF ELECTRO-CHEMO-MECHANICAL DYNAMICS AND AGING IN LI-ION AND ALL-SOLID-STATE BATTERIES THROUGH CONTINUUM MULTIPHYSICS MODELLING

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Abstract of the PhD research

Energy is the backbone of modern society, driving transportation system, industrial production, global communication, and advanced technology. For over a century, fossil fuels, such as coal, oil, and natural gas, have been the dominant sources driving global progress. However, their extensive use releases large amounts of carbon dioxide (CO_2), the main greenhouse gas that accelerates climate change. To mitigate environmental impact and ensure a sustainable future, there is a worldwide push to transition toward cleaner and more efficient energy systems. Lithium-ion batteries (LIBs) are currently the most promising energy storage solutions for this transformation, powering electric vehicles, portable electronics, and grid storage systems worldwide. However, their internal materials and interfaces gradually degrade owing to the complex (electro)chemical and physical changes that occur inside the battery during repeated use. This degradation causes capacity fading and efficiency loss, imposing fundamental limits on battery performance and lifetime. Understanding and quantifying these aging processes is crucial for designing more reliable, safer, and longer-lasting batteries for affordable, widespread clean energy storage.

This thesis focuses on developing an advanced continuum modeling framework, supported by experimental measurements, to analyze and predict battery performance and degradation under realistic conditions. The study was applied to both conventional LIBs with liquid electrolytes and emerging all-solid-state LIB systems. The study progresses methodologically from simplified multiphysics descriptions and material structures to complex electrode geometries, with experimental validation at each development stage.

This approach advances through two integrated phases. First, an impedance spectroscopy digital twin is developed that converts experimental EIS measurements into material aging parameters, enabling accurate capacity-loss forecasting across the lifecycle of conventional Li-ion cells. Second, the continuum modeling framework was extended to solid-state batteries, demonstrating that electrochemistry-mechanics coupling and state-dependent material properties are crucial for realistic lifetime prediction. This study identifies three critical factors that govern performance and lifetime: multiphysics interactions between chemistry and mechanics, parameter assumptions that reflect evolving material properties, and electrode geometries that create stress concentrations that drive cracking and capacity fading. Through this study, experimentally validated structure-property-performance relationships are established, advancing predictive modeling beyond the current state-of-the-art capabilities.

Overall, the multiscale framework provides both fundamental mechanistic insights and practical design guidance for material and electrode structure optimization. These advances help to accelerate the development of safer and longer-lasting batteries, which are essential for large-scale electrification and the global energy transition.