Abstract

Modern engineering components and systems increasingly require materials whose structural reliability, electromechanical response, and interfacial stability are specified together with their geometry and operating conditions. Grounded in material characterisation and modelling, this dissertation develops computational methodologies for predicting material response and relating it to component-, device-, and system-level requirements. The studied systems include multicomponent alloys, piezoelectric ceramics and polymers, and lithium-based battery interfaces. Their behaviour emerges from descriptors that span atomic bonding, crystal symmetry, microstructure, and interfacial morphology. No single modelling approach covers this full range of scales. The proposed scale-bridging framework therefore combines physics-based modelling with data-driven methods. It connects material descriptors to structural and functional response through an explicit intermediate material state.

In multicomponent alloys, ensemble machine learning supports structural alloy specification by mapping composition and manufacturing route jointly to the hardness-elongation balance and identifying coupled design regions rather than isolated optima. DFT-calibrated phase-field simulations indicate that matching elastic constants to the simulation temperature changes the predicted Al-Cu-Ni microstructure by 18%. This result confirms that temperature consistency is necessary for microstructure prediction relevant to process and component design. In piezoelectric materials, a crystallography-informed network predicts the complete symmetry-constrained piezoelectric tensor and evaluates it in a finite element device model. A model-identified doped-AlN composition, evaluated at an optimised orientation, raises the predicted energy-harvesting output 9.96-fold relative to the undoped baseline. A complementary physics-guided model links electrospinning conditions and filler content to the effective response of PVDF/SnO_2 nanofibres and raises the predicted d_{33} from 18 to 29 pC N^{-1}. In lithium-based battery interfaces, a coupled-field phase-field model resolves the tip-amplified mechanism of dendrite growth. A literature synthesis consolidates materials, interfacial, and operating suppression strategies into ten jointly constrained performance and stability targets for reliable electrochemical energy systems.

Across all three domains, a common design logic recurs even though the governing physics and models differ by material. Composition and processing define the attainable response. The intermediate material state carries this information to the component, device, or interface. At that level, coupled multi-physics behaviour determines the realised performance. These findings are distilled into five transferable schemes for structural alloy components, piezoelectric sensors and energy harvesters, and electrochemical energy systems.