Silesian University of Technology
Faculty of Mechanical Engineering
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Extended Abstract

Scale Bridging Computational and Data-Driven Design of Microstructures in Multicomponent Alloys for Advanced Functional Materials

Doctoral Dissertation

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M.Sc., Eng.

Scientific discipline: Mechanical Engineering

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Structure of the Extended Abstract

Dissertation Title

The title of the dissertation is:

Scale Bridging Computational and Data-Driven Design of Microstructures in Multicomponent Alloys for Advanced Functional Materials

Engineering Scope and Research Subject

This dissertation develops computational methods for designing and assessing components whose performance depends on material response during processing and service. The work is not limited to describing materials. Material behaviour is studied because it affects load capacity, electromechanical output, interfacial stability, durability, reliability, and service performance.

The research addresses three connected design contexts. The first is the specification of multicomponent alloys for structural and functional components. The second is the prediction of electromechanical response in sensors, actuators, MEMS devices, and energy harvesters. The third is the reliability of lithium-based battery interfaces, where stable operation depends on controlling interfacial damage and dendrite growth.

Across these contexts, the central task is to connect material descriptors with component performance. For alloys, the descriptors include composition, processing route, elastic constants, and grain morphology. For piezoelectric systems, they include crystal symmetry, tensor components, orientation, filler content, phase fraction, and fibre morphology. For lithium-based interfaces, they include concentration fields, electric-potential fields, interface shape, and operating conditions.

A scale-bridging logic links these descriptors to engineering assessment. Composition and processing define an intermediate material state. This state may be a microstructure, an oriented tensor, a fibre morphology, or an evolving interface. It carries lower-scale information to the component, device, or system level. Computational mechanics and finite element analysis are then used to evaluate performance under operating conditions.

Although interdisciplinary, the work remains design oriented. It uses materials data, atomistic calculations, phase-field simulation, machine learning, and finite element analysis to support engineering decisions. These decisions include selecting alloy and process windows, choosing and orienting active materials, and defining reliability targets for electrochemical systems.

Objectives and Theses

The overall objective is to develop and apply computational methods that combine physics-based modelling with data-driven prediction. The methods connect descriptors and intermediate material states with structural and functional performance. In this way, they support alloy and

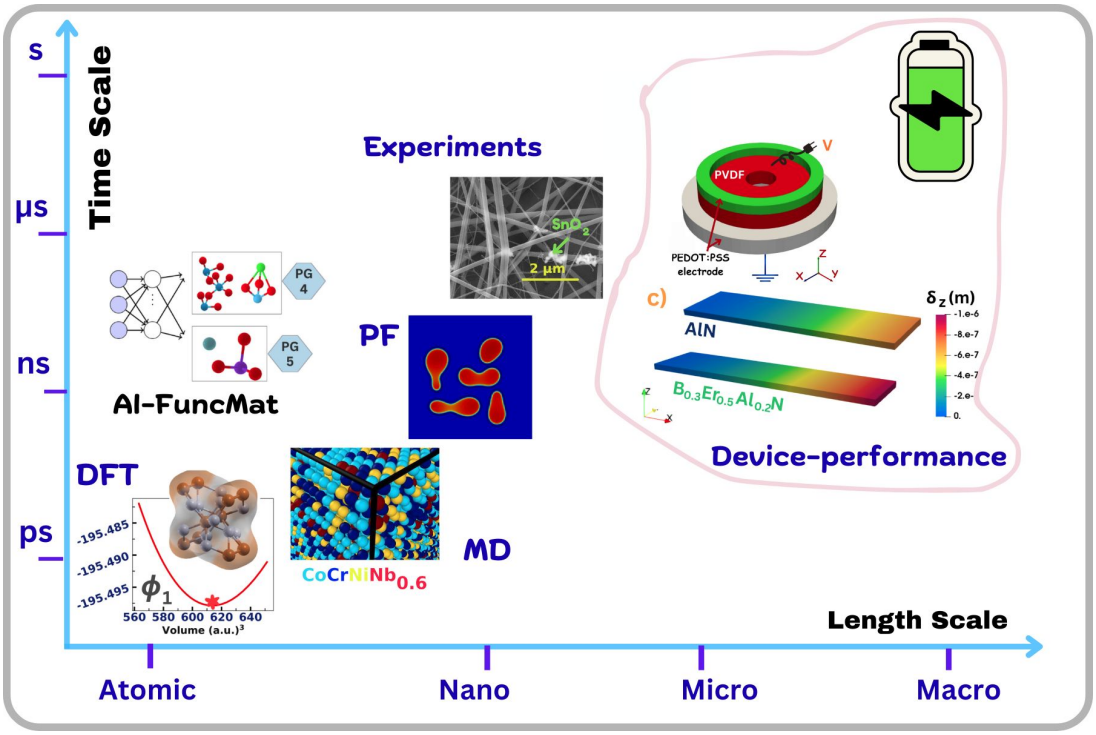

Figure 1: Scale-bridging logic used in the dissertation. Lower-scale descriptors are connected to intermediate states, and these states are then evaluated at component, device, or interface scale.

process selection, piezoelectric device design, and reliability assessment of electrochemical energy systems.

The dissertation has three specific objectives:

1. To develop scale-bridging alloy models that support material and process specification for components exposed to mechanical or functional service requirements.
2. To model piezoelectric performance for sensor, actuator, and energy-harvester components.
3. To evaluate dendritic instability in lithium-based interfaces and define design targets for durability, reliability, and safe operation.

The central thesis states that a scale-bridging framework can create reliable descriptor-to-performance pathways across different material classes and component types. This does not require one universal model. It requires meaningful descriptors, consistent transfer of parameters across scales, and explicit representation of the intermediate material state.

The supporting theses are design oriented. Coupled physics-based and data-driven modelling can provide capabilities that neither approach provides alone. Composition-route descriptors can identify balanced alloy design regions for load-bearing performance. Temperature-calibrated elastic tensors can strengthen mesoscale process simulation. Full-tensor and morphology-based models can guide piezoelectric component design. Coupled-field simulation can explain dendrite growth and organise suppression strategies into reliability targets.

Table 1: Objectives, research problems, and design evidence.

Objective	**Research problem**	**Design evidence**
Alloy and process specification	Composition, processing, and microstructure are often treated separately.	Hardness-elongation prediction, inverse design windows, and temperature-calibrated phase-field simulations.
Piezoelectric component design	Scalar coefficients do not capture tensor anisotropy, morphology, orientation, or device constraints.	Symmetry-consistent tensor prediction, finite element evaluation, and processing-aware polymer models.
Battery-interface reliability	Dendrite growth depends on coupled transport, electrical, and interfacial fields.	Phase-field dendrite simulation and a multi-metric durability and reliability roadmap.

Computational Design Workflow

The dissertation combines four groups of methods. Together, they support the process-to-performance chain.

Data-driven models provide rapid property prediction. AlloyManufacturingNet maps alloy composition and manufacturing route to the hardness-elongation balance needed for structural specification [P-I]. PiezoTensorNet predicts the complete symmetry-constrained piezoelectric tensor for device-oriented evaluation [P-II]. PGMLpiezo predicts the effective response of PVDF/SnO_2 nanofibres from processing and morphology descriptors [P-V].

Atomistic and first-principles calculations supply lower-scale parameters. Density functional theory provides elastic tensors for Al-Cu-Ni phase-field simulations [P-III]. Molecular dynamics nanoindentation links Nb addition in $CoCrNiNb_x$ to local deformation resistance [P-I].

Phase-field simulations describe evolving intermediate states. A DFT-informed model predicts Al-Cu-Ni phase evolution during process-relevant thermal conditions. A coupled-field model describes lithium deposition and dendrite growth. In both cases, an evolving interface or microstructure acts as the intermediate state.

Finite element simulations evaluate whether predicted material changes lead to useful device-level performance. They are used for oriented AlN piezoelectric beams and PVDF/SnO_2 flexible devices.

Alloy Process Design and Structural Performance

The alloy studies demonstrate that composition and manufacturing route should be specified together for structural performance. Composition alone does not determine the final mechanical response. Processing defines the intermediate state, which controls properties under load.

AlloyManufacturingNet predicts hardness and elongation using composition and manufacturing-route descriptors [P-I]. A scale-invariant objective function is used to identify balanced design regions. This avoids selecting a composition that improves one property while reducing the other.

The predictions indicate that ZrHfNb-derived systems have separated high-hardness and high-ductility regions. VNbTa-derived systems have a broader balanced design window. Promising regions include $Mo_{0.3}(VNbTa)_{0.7}$ and selected Cr-W modified candidates.

The $CoCrNiNb_x$ study tests the trend along one composition axis. Increasing Nb raises hardness. Elongation first decreases and then partly recovers. The balanced region is located near $CoCrNiNb_{0.6}$. Molecular dynamics nanoindentation indicates that the Nb-containing slab resists penetration more strongly than CoCrNi. This connects the property trend to a nanoscale deformation mechanism.

The Al-Cu-Ni phase-field study adds the process-scale part of the same design chain [P-III]. It transfers phase-specific elastic constants from DFT into a mesoscale phase-field model. Elastic constants calibrated at 723 K change the predicted grain area by 18.18% compared with 0 K inputs. This result supports using process simulations with parameters that match the manufacturing temperature.

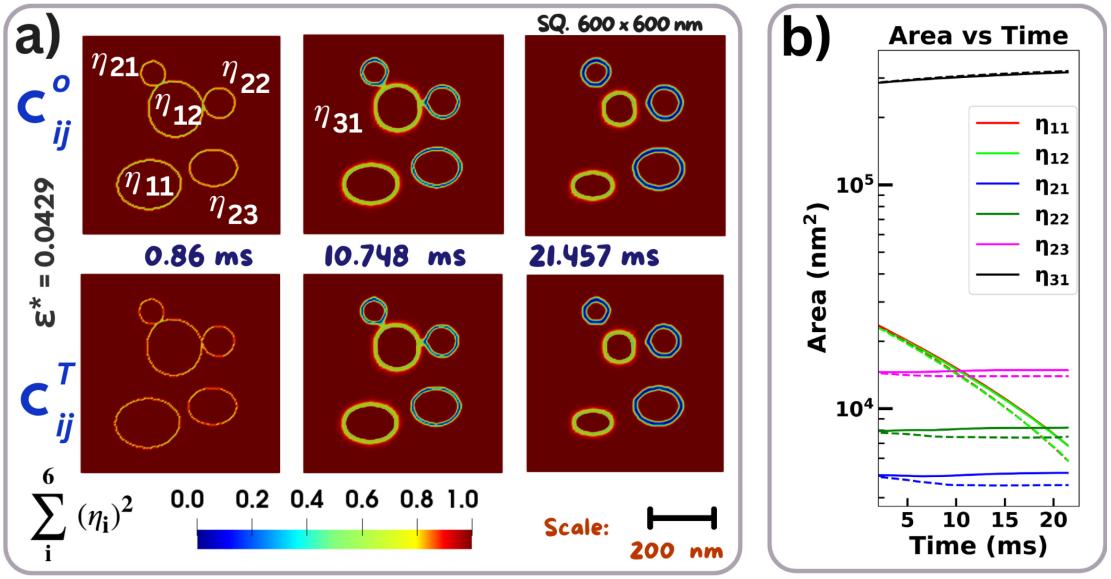

Figure 2: Temperature-calibrated phase-field simulation of Al-Cu-Ni microstructure evolution. The figure illustrates that elastic parameters affect predicted morphology during process-relevant simulation.

The corrosion study on additively manufactured super duplex stainless steel extends the composition-processing logic to surface durability [P-VI]. It uses heat-treatment and composition descriptors to support corrosion-resistance assessment in LPBF-processed components. The post-processing study further links heat-treatment routes to strength and toughness response [P-VII].

Piezoelectric Device Performance

The piezoelectric studies demonstrate that scalar coefficients are insufficient for component design. Device output depends on the full tensor, orientation, elastic and dielectric properties, geometry, boundary conditions, and the external circuit.

PiezoTensorNet predicts the full symmetry-constrained piezoelectric tensor [P-II]. A point-group classifier routes each candidate to a symmetry-specific regression module. The model predicts only the tensor components allowed by symmetry. This prevents unphysical tensor outputs and allows tensor rotation into the device frame.

The screening identifies B-Er co-doped AlN as a leading candidate for device-level evaluation. Near $B_{0.3}Er_{0.5}Al_{0.2}N$, the tensor norm e_{mod} reaches 4.37 C m^{-2}. The value for undoped AlN is 1.67 C m^{-2}. Tensor rotation identifies favourable orientations. A finite element beam simulation indicates that the optimised and oriented candidate can increase simulated harvester power by 9.96 times relative to the undoped baseline.

The PVDF/SnO_2 study addresses flexible piezoelectric devices with limited data [P-V]. It links electrospinning settings, filler content, fibre diameter, phase fraction, and effective piezoelectric response. The predicted d_{33} increases from 18 to 29 pC N^{-1} under optimised fabrication conditions.

Finite element simulations demonstrate that device architecture also affects the realised response. Passive harvesting gives an average power of 0.359 nW. A P-SSHI conditioning circuit raises the average power to 1.251 nW. In actuator mode, lateral constraints increase axial stroke from 44.41 nm to 69.60 nm. The increase is about 57%. These results support joint design of processing, morphology, circuits, and boundary conditions.

Battery-Interface Reliability

The battery-interface study focuses on reliability of lithium-based energy systems [P-IV]. Dendrites can consume active material, damage the interface, and cause short circuits. Their growth depends on coupled transport, electrical, and interfacial fields.

The phase-field model treats the lithium-electrolyte boundary as an evolving diffuse interface. The order parameter, concentration field, and electric potential field are solved together. A small protrusion localises the fields. Deposition then accelerates at the tip. The growing tip further

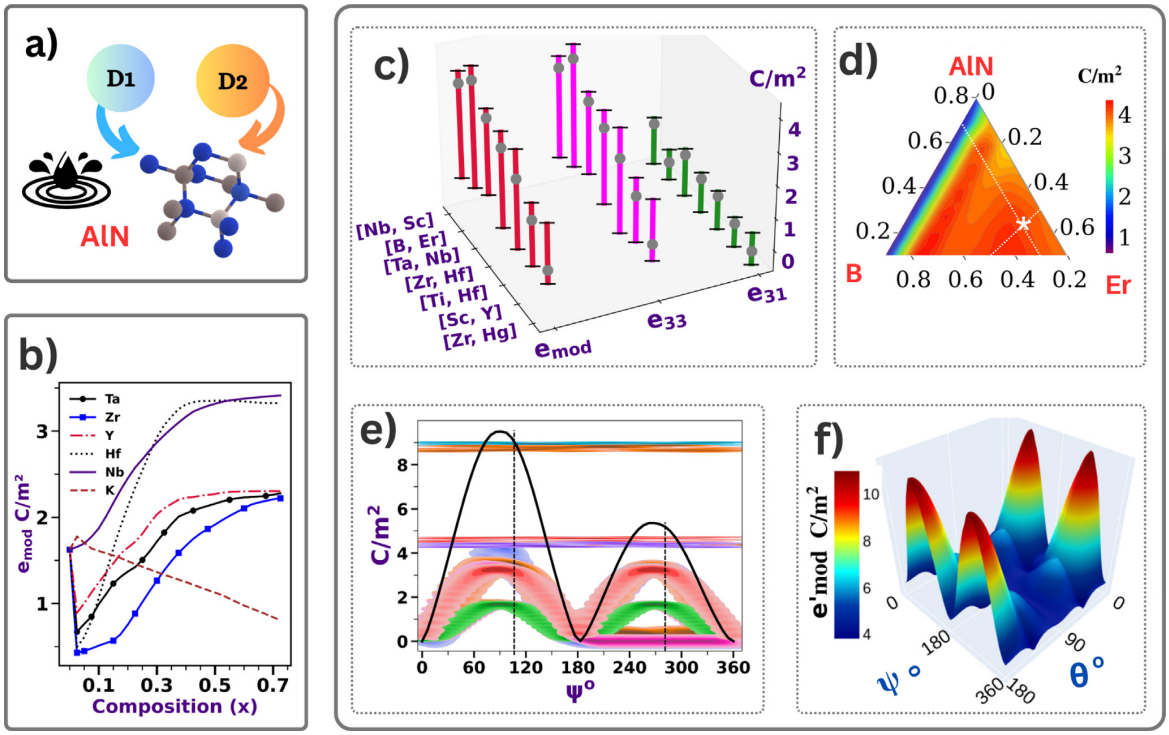

Figure 3: PiezoTensorNet design sequence for doped AlN. Chemistry changes the tensor, tensor rotation changes the projected response, and finite element analysis evaluates the device-level output.

intensifies the local driving forces. This creates a self-amplifying feedback between geometry, transport, and electrochemical deposition.

The roadmap study translates this mechanism into design targets [P-IV]. It groups material, interfacial, and operating strategies into ten coupled metrics. These metrics include transport, stiffness, current density, efficiency, defect density, capacity retention, and temperature-related stability. This framing treats dendrite suppression as a joint design envelope.

Prospective Active Component Screening

The dissertation also includes a prospective screening study. Alloy-derived cation pools are reused to search oxide and nitride chemistries for electromechanical, dielectric, and polar responses. This study narrows the search space for future active component design, but it is not presented as a validated material design result.

The screening combines transition-metal cation spaces with symmetry rules from the tensor study. Nb-Ti-Zr and Nb-Ta-Ti oxide regions emerge as leading candidates. The maps also reveal trade-offs. A wider band gap tends to accompany lower spontaneous polarisation. Electromechanical response tends to saturate at high permittivity. The useful result is a balanced Pareto window rather than a single-property maximum.

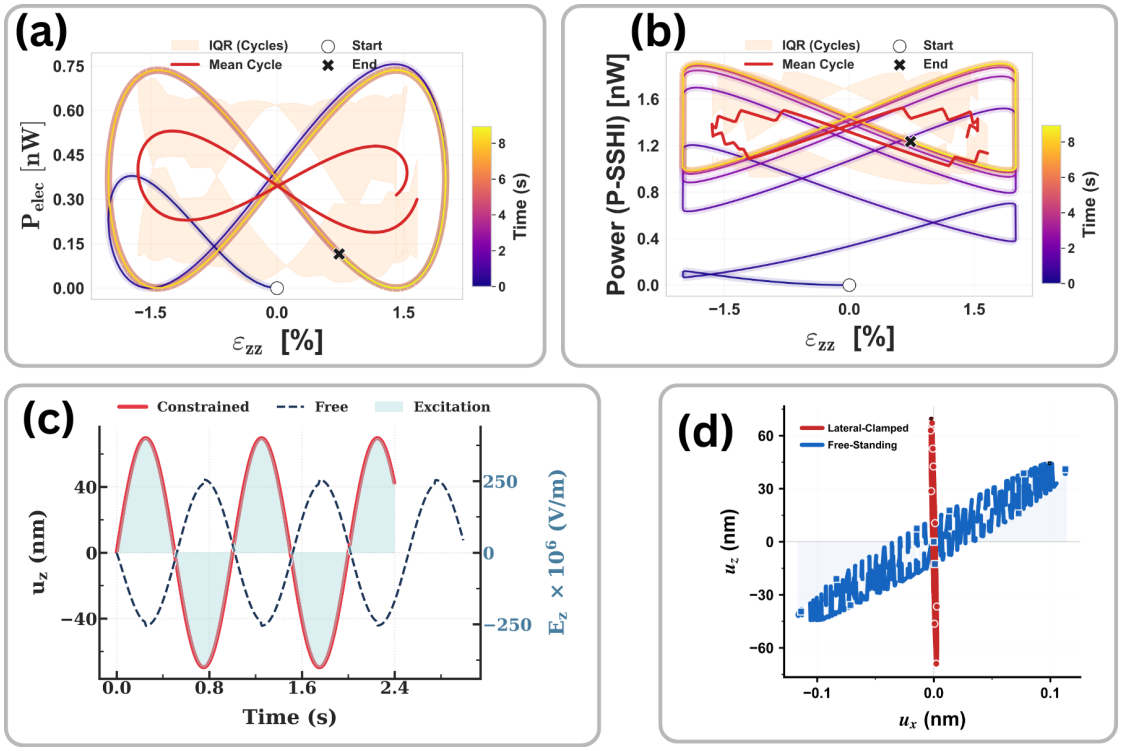

Figure 4: PVDF/SnO_2 finite element simulations. Electrical conditioning increases harvested power. Mechanical constraints increase useful actuator stroke.

Conclusions

The dissertation demonstrates that material behaviour can be used directly in computational design workflows when lower-scale descriptors are linked to component performance through an explicit intermediate state.

For alloys, chemistry and processing must be specified together. The hardness-elongation balance cannot be predicted reliably from composition alone. Temperature-consistent elastic tensors are also important because they change predicted microstructure during process simulation.

For piezoelectric components, full tensor information is needed for design. Symmetry, orientation, morphology, boundary conditions, and circuits jointly determine realised output.

For battery interfaces, dendrite suppression must address coupled fields. Reliable operation requires combined targets for materials, interfaces, manufacturing quality, and operating conditions.

Across all domains, the contribution is a set of computational pathways that convert material information into performance prediction. These pathways support component specification, service-performance assessment, and reliability-oriented design without treating material characterisation as an isolated objective.

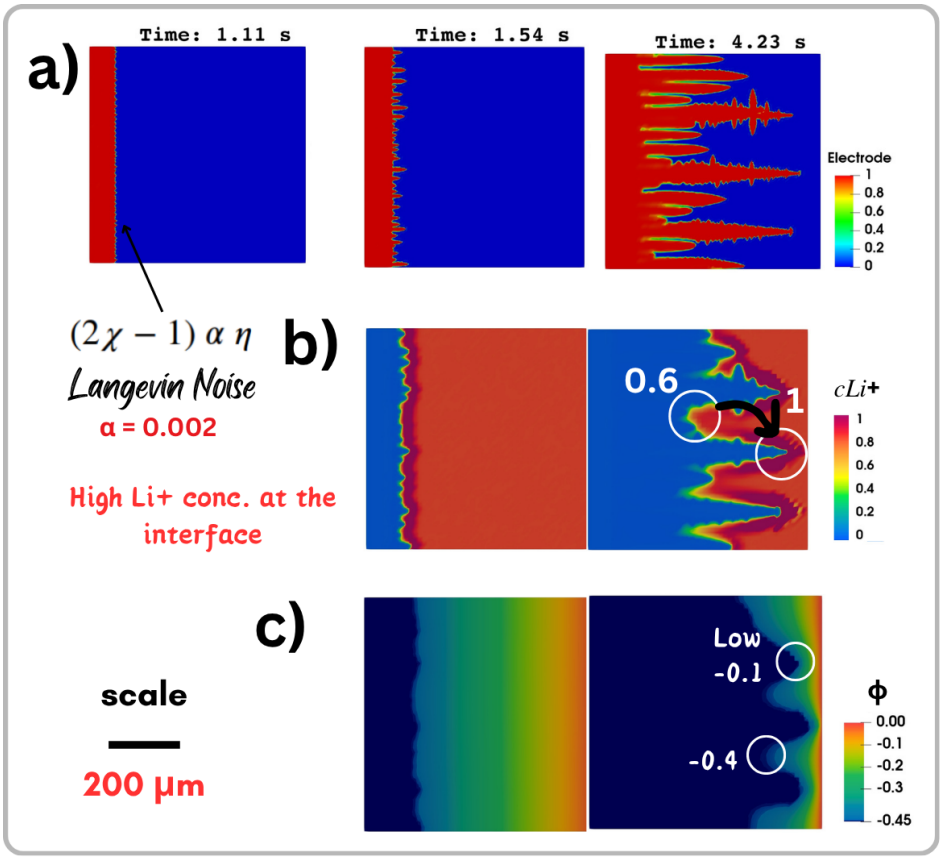

Figure 5: Coupled-field simulation of lithium dendrite growth. Local field concentration at protruding tips drives non-uniform deposition and interface instability.

List of Publications

This publication-based dissertation is based on seven peer-reviewed journal articles. The candidate's contributions are summarised after the publication list, and the signed co-author declarations are included in the dissertation documentation.

[P-I] **S. Poudel**, U. Subedi, M. O. Hamid, K. Gyanwali*, N. Moelans, A. Timofiejczuk, and A. Kunwar*, "AlloyManufacturingNet for discovery and design of hardness-elongation synergy in multi-principal element alloys," *Engineering Applications of Artificial Intelligence*, vol. 132, p. 107902, 2024.
DOI: 10.1016/j.engappai.2024.107902
(IF: 9.0, MNiSW: 140)#

[P-II] **S. Poudel***, R. Thapa, R. Basnet, A. Timofiejczuk, and A. Kunwar, "PiezoTensorNet: Crystallography informed multi-scale hierarchical machine learning model for rapid piezoelectric performance finetuning," *Applied Energy*, vol. 361, p. 122901, 2024.
DOI: 10.1016/j.apenergy.2024.122901
(IF: 12.2, MNiSW: 200)

[P-III] **S. Poudel***, N. Moelans, R. Thapa, A. Timofiejczuk, D. Panthi, and A. Kunwar, "Unraveling elastochemical effects in microstructural evolution of Al–Cu–Ni system through DFT-informed multi-phase field simulations," *International Journal of Solids and Structures*, vol. 300, p. 112894, 2024.
DOI: 10.1016/j.ijsolstr.2024.112894
(IF: 4.6, MNiSW: 140)

[P-IV] Y. Li, **S. Poudel***, S. Kumari, E. Azqadan, A. Kunwar*, and N. Moelans*, "Roadmaps for dendrite suppression in next generation lithium-ion batteries: Toward sustainable energy solutions," *Energy Storage Materials*, vol. 86, p. 105000, 2026.
DOI: 10.1016/j.ensm.2026.105000
(IF: 19.3, MNiSW: 200)

[P-V] **S. Poudel***, W. Smok, R. Thapa, A. Timofiejczuk, N. Moelans, and A. Kunwar, "Physics-guided machine learning for enhanced piezoelectric performance in electrospun PVDF/SnO_2 nanofibers," *Sustainable Materials and Technologies*, p. e02008, 2026.
DOI: 10.1016/j.susmat.2026.e02008
(IF: 9.7, MNiSW: 200)

[P-VI] M. Dagnaw, **S. Poudel***, U. Subedi*, R. Thapa, Ł. Reimann, A. N. S. Appiah, P. M. Nuckowski, M. Król, Z. Brytan, N. Moelans, et al., "Integrating experiments and phase field method through

informatics for tailored corrosion performance of additively manufactured steel microstructures," *Metals and Materials International*, 2026.
DOI: 10.1007/s12540-026-02369-4
(IF: 4.5, MNiSW: 70)

[P-VII] M. Dagnaw, **S. Poudel***, M. Król, and Z. Brytan, "Post-process heat treatment design for tunable strength and toughness in L-PBF 2507 super duplex stainless steel," *Materialia*, p. 102799, 2026.
DOI: 10.1016/j.mtla.2026.102799
(IF: 3.1, MNiSW: 20)

Additional Related Publications

The following publications provide complementary methodological context for the dissertation.

[AP-I] R. Thapa, **S. Poudel**, K. Krukiewicz, and A. Kunwar*, "A topical review on AI-interlinked biodomain sensors for multi-purpose applications," *Measurement*, vol. 227, p. 114123, 2024.
DOI: 10.1016/j.measurement.2024.114123
(IF: 6.1, MNiSW: 200)#

[AP-II] S. Neupane*, **S. Poudel***, A. Ghimire, and S. Shakya, "Enhanced mechanical performance and biodegradability in filler-reinforced potato biopolymers for sustainable packaging," *Materials Today Communications*, p. 114081, 2025.
DOI: 10.1016/j.mtcomm.2025.114081
(IF: 4.9, MNiSW: 70)

* Corresponding author.

IF: Impact Factor (2025 values). MNiSW: Polish Ministry of Science and Higher Education points score.

Author's Contribution

This chapter summarises the role of the candidate (**Sachin Poudel**) in each of the seven publications. It reports publication position, percentage contribution, CRediT roles, and the principal tasks completed by the candidate. The signed contribution declarations are included in the dissertation documentation.

Publication I [P-I]

Position: First. **Contribution:** 51%.

CRediT roles: Conceptualization, methodology, software, investigation, formal analysis, validation, data curation, visualization, funding acquisition, writing: original draft.

- Framed structural alloy specification as a joint choice of composition and manufacturing route for hardness-elongation requirements.
- Enabled prediction and inverse design using curated multi-route data and the scale-invariant objective $F(x,y)$.
- Used physically grounded descriptors (ΔB, ΔG, VEC) to retain mechanical interpretation.
- Linked predicted property trends to atomistic deformation mechanisms through $CoCrNiNb_x$ molecular-dynamics nanoindentation and led the manuscript, figures, and funding.

Publication II [P-II]

Position: First and Corresponding. **Contribution:** 61%.

CRediT roles: Conceptualization, methodology, software, investigation, formal analysis, validation, data curation, visualization, writing: original draft.

- Supported sensor and energy-harvester material selection by connecting complete symmetry-constrained piezoelectric tensors to oriented finite element device models.
- Ensured physically admissible tensor outputs using a hierarchical point-group classifier, symmetry-specific regressors, crystallographic descriptors, and the tensor-norm screening metric e_{mod}.
- Identified B-Er co-doped AlN as the leading MEMS energy-harvesting candidate, demonstrated a 9.96-fold predicted power gain, and led the writing and figures.

Publication III [P-III]

Position: First and Corresponding. **Contribution:** 65%.

CRediT roles: Conceptualization, methodology, software, investigation, formal analysis, validation, data curation, visualization, writing: original draft.

- Treated Al-Cu-Ni phase evolution as a process-design problem requiring temperature-consistent microstructure prediction.
- Enabled temperature-consistent mesoscale simulation by implementing a DFT-informed MOOSE phase-field model and transferring calibrated elastic constants.
- Quantified the 18% morphology difference relative to 0 K parameters, established the atomistic-to-mesoscale transfer procedure, and led the writing, figures, and interpretation.

Publication IV [P-IV]

Position: Second and Corresponding. **Contribution:** 35%.

CRediT roles: Methodology, investigation, formal analysis, validation, visualization, writing: review & editing.

- Formulated reliability targets for lithium-based energy systems by co-developing a dendrite-suppression roadmap.
- Mapped degradation mechanisms to materials, interfacial, and operating strategies.
- Organised dispersed suppression approaches into ten coupled performance and stability metrics for design assessment.
- Co-wrote the modelling and battery-interface sections, prepared figures, and integrated phase-field insights into the roadmap narrative.

Publication V [P-V]

Position: First and Corresponding. **Contribution:** 50%.

CRediT roles: Conceptualization, methodology, software, investigation, formal analysis, validation, data curation, visualization, project administration, funding acquisition, writing: original draft.

- Framed flexible sensor, actuator, and energy-harvester design under sparse data.
- Connected electrospinning conditions, SnO_2 content, morphology, and effective PVDF response.
- Converted dispersed literature data into a structured modelling dataset using literature mining and processing-aware descriptors.
- Evaluated predicted d_{33} improvements through FERRET device simulations and led the writing, project administration, figures, and funding.

Publication VI [P-VI]

Position: Second and Corresponding. **Contribution:** 14%.

CRediT roles: Conceptualization, methodology, software, data curation, visualization, writing: review & editing.

- Extended corrosion-performance specification for LPBF-processed SDSS 2507 through composition-processing modelling.
- Represented heat-treatment and composition interactions through process-sensitive descriptors, including PREN-temperature and $T \times t$ features, within the Matminer/Magpie workflow.
- Contributed to SPER-based phase-stability representation, data curation, validation, figures, and interpretation.

Publication VII [P-VII]

Position: Second and Corresponding. **Contribution:** 25%.

CRediT roles: Conceptualization, software, formal analysis, data curation, visualization, writing: review & editing.

- Guided post-processing selection for L-PBF 2507 components by linking heat-treatment routes to strength-toughness response.
- Provided the analysis software and curated dataset used for process-selection interpretation, figures, and manuscript revision.