C1 — Project Description

DRAFT - Dr Yuefeng Yin - FT26 baseline for FT27 review

PROJECT TITLE

Beyond Order: Disorder-Oriented Design of Quantum Materials

PROJECT QUALITY AND INNOVATION

Background and Project Aims

The advancement of modern technology is fundamentally driven by discovering and designing new material systems. This is clearly reflected in many Nobel Prizes awarded in this century. Graphene has revolutionised flexible electronics and high-speed transistors through its exceptional conductivity and mechanical strength. Lithium-ion battery materials have transformed portable electronics and enabled the rise of electric vehicles through efficient energy storage. Topological insulators have opened pathways to low-power spintronic and quantum-computing devices by exploiting robust surface states. Metal–organic frameworks have advanced gas capture, catalysis, and biomedical sensing through their high porosity and chemical tunability. These breakthroughs demonstrate how materials innovation drives technological progress across diverse industries.

At the heart of this materials-driven progress lies the semiconductor industry, which powers the information and communications technology (ICT) revolution—arguably the most transformative technological development in modern history. The industry, worth over USD 600 billion annually, has produced more than 10^{21} transistors, forming the backbone of global computing and connectivity. For nearly five decades, this growth has relied on silicon-based complementary metal–oxide–semiconductor (CMOS) technology, whose predictable scaling enabled faster, smaller, and more energy-efficient devices under Moore's law. Yet, as transistor dimensions approach atomic limits, further improvements have become prohibitively difficult and costly. With information technology already consuming nearly 8% of global electricity and demand accelerating due to artificial intelligence and data-intensive applications, the need for new materials is more urgent than ever. **Future progress in semiconductor innovation will depend on materials that can deliver transformative gains in energy efficiency, scalability, and functionality.**

This project aims to establish a new design framework that redefines disorder as a controllable and useful feature in materials science. Disorder, in this context, extends beyond structural irregularities to include electronic, magnetic, and interfacial variations that can fundamentally alter a material's physical properties. Rather than suppressing these irregularities, this project will harness the power of disorder to design next-generation materials for energy-efficient and sustainable electronics. Specifically, the aims of this fellowship are to:

1. Develop advanced computational methods that integrate density-functional theory and artificial intelligence to predict how different forms of disorder—structural, electronic, and magnetic—affect material stability and transport behaviour.
2. Discover and model new classes of disorder-engineered materials with tunable electronic and spintronic properties suitable for next-generation chips and quantum devices.
3. Establish a quantitative framework linking disorder characteristics to measurable device performance, guiding experimental realisation and integration with existing semiconductor technologies.
4. Create a digital platform for disorder-oriented materials design, enabling rapid screening, reproducibility, and community-driven innovation.

The outcome of this fellowship will provide: (1) A new scientific foundation and knowledge framework for understanding how structural, electronic, and magnetic disorders can be purposefully engineered to enhance material functionality; (2) Advanced computational theories that quantitatively describe the interplay between disorder, stability, and electronic transport; (3) A materials design platform capable of predicting and optimising disorder-enabled materials for low-energy and quantum electronic applications, and (4) Validated candidate materials with demonstrated potential for integration into next-generation semiconductor and spintronic devices. The success of this fellowship will open new avenues for energy-efficient materials discovery and accelerate Australia's leadership in sustainable semiconductor innovation and advanced manufacturing.

Through achieving these objectives, the fellowship will transform disorder from a challenge into a powerful design principle, opening new avenues for materials discovery and advancing Australia's

leadership in computational materials innovation and semiconductor research.

Innovation in the Context of Recent International Advances in this Area

The global semiconductor and quantum materials community is undergoing a rapid transformation driven by the urgent need to overcome the physical and scaling limits of silicon. Around the world, researchers are developing new material systems and device architectures that promise faster operation and reduced power consumption. Transition metal dichalcogenides (TMDs), topological insulators, and two-dimensional oxides have emerged as strong contenders for next-generation electronics, offering ultrathin geometries, tunable bandgaps, and unique spin–orbit interactions. In the past year, several leading research groups in the United States, Europe, and Asia have demonstrated high-mobility TMD transistors and hybrid quantum devices that outperform conventional silicon-based platforms. These achievements have accelerated global competition toward developing materials that can sustain the exponential growth of computational demand while drastically reducing energy use.

Out of these advances, a clear trend is emerging toward incorporating disorder as a controllable design parameter in material synthesis and device fabrication. As illustrated in the left panel of Fig. 1, disorder effects can be utilised in several ways: (a) Employing disordered (amorphous) materials directly as the channel layer to achieve performance comparable to crystalline counterparts, but at significantly lower assembly cost; (b) Combining disorder with external fields or strain to create reconfigurable electronic behaviour, thereby realising the low-energy advantages of quantum materials; and (c) Introducing controlled disorder at heterostructure interfaces to facilitate the growth of high-quality crystalline layers, as recently demonstrated for MX_2 systems. Consequently, disorder effects have become an essential element in semiconductor technology development, with an increasing number of innovations now emerging from this strategy.

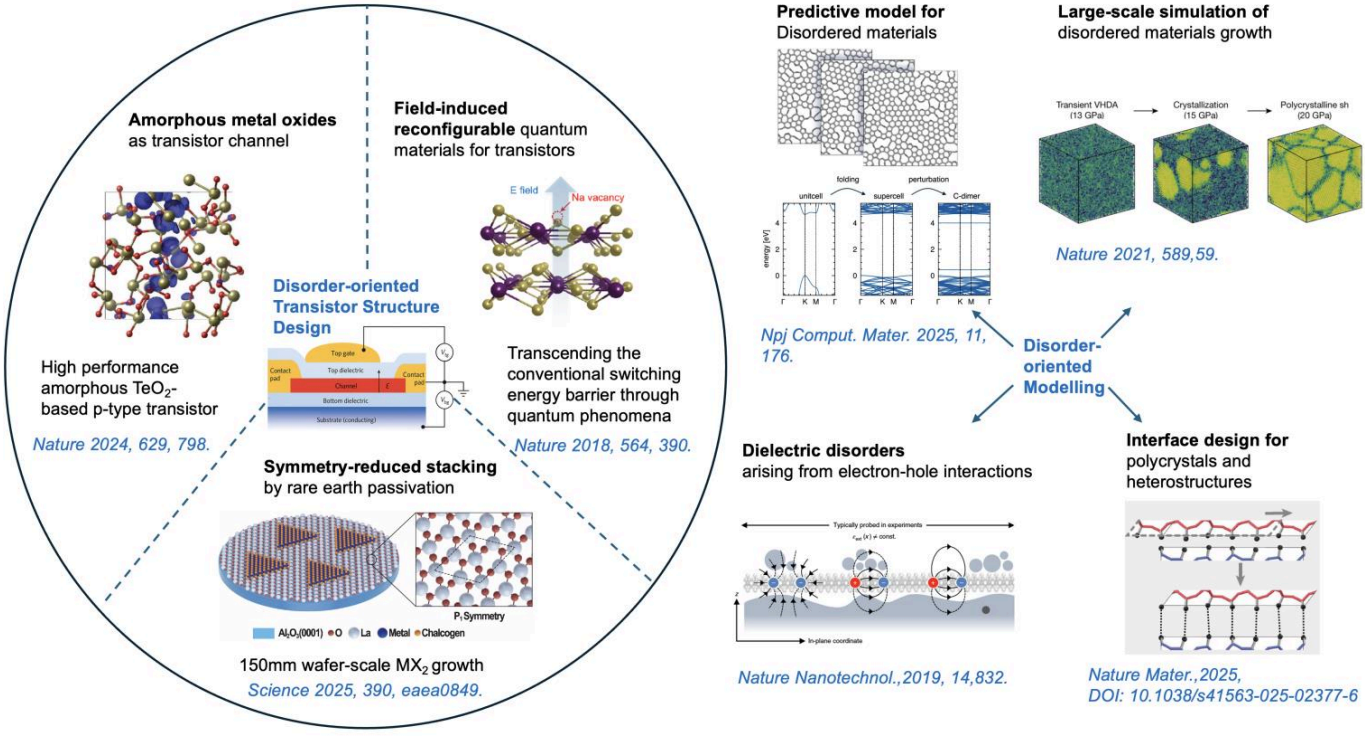

Figure 1. (Left) Recent significant advances in transistor structure design that incorporate disorders as key elements. (Right) Key topics for disorder-oriented modelling.

Computational and theoretical approaches are indispensable for investigating disorder effects. The right panel of Fig. 1 highlights how computational modelling has advanced materials design involving disorder. The main research interests include: (a) Developing predictive models for generating disordered materials to quantify the influence of disorder on electronic structure; (b) Performing large-scale dynamic simulations of the growth processes in disordered materials, including polycrystalline and amorphous systems; (c) Studying how disorder at material interfaces can stabilise growth or modify electronic transport; and (d) Exploring new sources of disorder arising from electronic and magnetic impurities. Given the strategic importance of understanding disorder and the inherent complexity of modelling it, disorder-oriented materials modelling is often regarded as the "final frontier" of materials design. Now with the emergence of machine learning and artificial intelligence, the vision of using computational modelling to guide materials design "by disorder" is becoming a realistic and achievable goal.

My previous and ongoing research, as shown in the box below, demonstrates my significant contributions to utilizing disorder effects to discover new materials and to enhance the electronic and spintronic structures of quantum materials. This fellowship will build upon the success of these investigations and draw inspiration from the current progress in the field to open a new chapter in "disorder-oriented materials design".

Box: My previous research progress related with "disorder-oriented materials design".

Npj. Quantum Mater. 2019, 4, 47.

I use local surface perturbations to first reveal anisotropic spin textures in the non-magnetic compound pyrite $OsSe_2$.

New J. Phys. 2021, 23, 063042; Mater Today Phys. 2023, 36, 101168; Mater Today Phys. 2025, 59, 101897.

My "Bismuth Trilogy" work establishes a computational framework, connecting DFT calculations to Wannier–TB models, to investigate the modification of electronic and spintronic structures through interfacial engineering and external electric fields.

Matter 2025, 8, 101988.

My computational modelling reveals the underlying physical mechanisms responsible for the giant Berry curvature observed experimentally in amorphous Co_2MnGa.

Patent Application US63/848,059

Recently, my collaboration with the Australian start-up TQ Transistors has revealed a new type of two-dimensional heterostructure incorporating disorders that significantly amplify the effect of an external electric field in manipulating the band gap of semiconductors. This setup offers the advantage of very low switching voltage and energy compared to current technology, while remaining feasible for large-scale production.

Research Question

Despite the promising potential revealed by recent breakthroughs, using disorder as a controllable factor remains highly challenging in practice. Ensuring that the exceptional performance achieved through the incorporation of disorder in transistor design occurs "by design" rather than "by coincidence" is critical for translating these research outcomes into viable chipmaking technologies. Computational modelling must play a key role by providing both physical insights and design principles to guide materials development for next-generation semiconductor technologies.

My previous experience in studying disorder in materials has raised several intriguing questions regarding the nature of disorder-enhanced performance in electronic devices, the controlled growth of disordered structures, and the refinement of methodologies for modelling disorder. In this fellowship, the following major research questions will be addressed in detail:

1. **Why can certain configurations of disorder enhance semiconductor performance, while others cannot?** This question concerns the fundamental problem of correlating the degree of amorphism in a crystal with the electronic structure of a material. Previous studies have shown that disordered structures exhibiting favourable device performance often contain "hidden" short-range order within overall randomness. Understanding how these local structural motifs influence charge transport and quantum states is essential for identifying which configurations of disorder are beneficial. A clear answer to this question will be critical for establishing a rational strategy to incorporate disorder into materials design for improved semiconductor performance.
2. **How can the growth of disordered structures be controlled?** While Question 1 focuses on static configurations, this question addresses the dynamic stability of disorder in materials. Disordered structures often exist in metastable states and can evolve under thermal, chemical, or mechanical perturbations. Controlling their growth and stabilisation requires understanding the thermodynamic and kinetic factors that govern disorder formation, as well as the effects of external parameters such as pressure, substrate, and electric field. Resolving this issue is essential for achieving reproducible fabrication and ensuring the long-term reliability of disorder-engineered materials in practical device environments.
3. **Is there a better and more efficient way to model disordered structures?** This methodological question focuses on improving the modelling of disorder effects and their correlation with external

fields or strains. Current approaches are often limited by specific constraints and scale gaps between different theoretical frameworks. A comprehensive computational framework is needed to integrate disorder modelling across multiple scales, providing reliable metrics that connect electronic structure to device-scale performance.

Project Design: Conceptual Framework and Approach

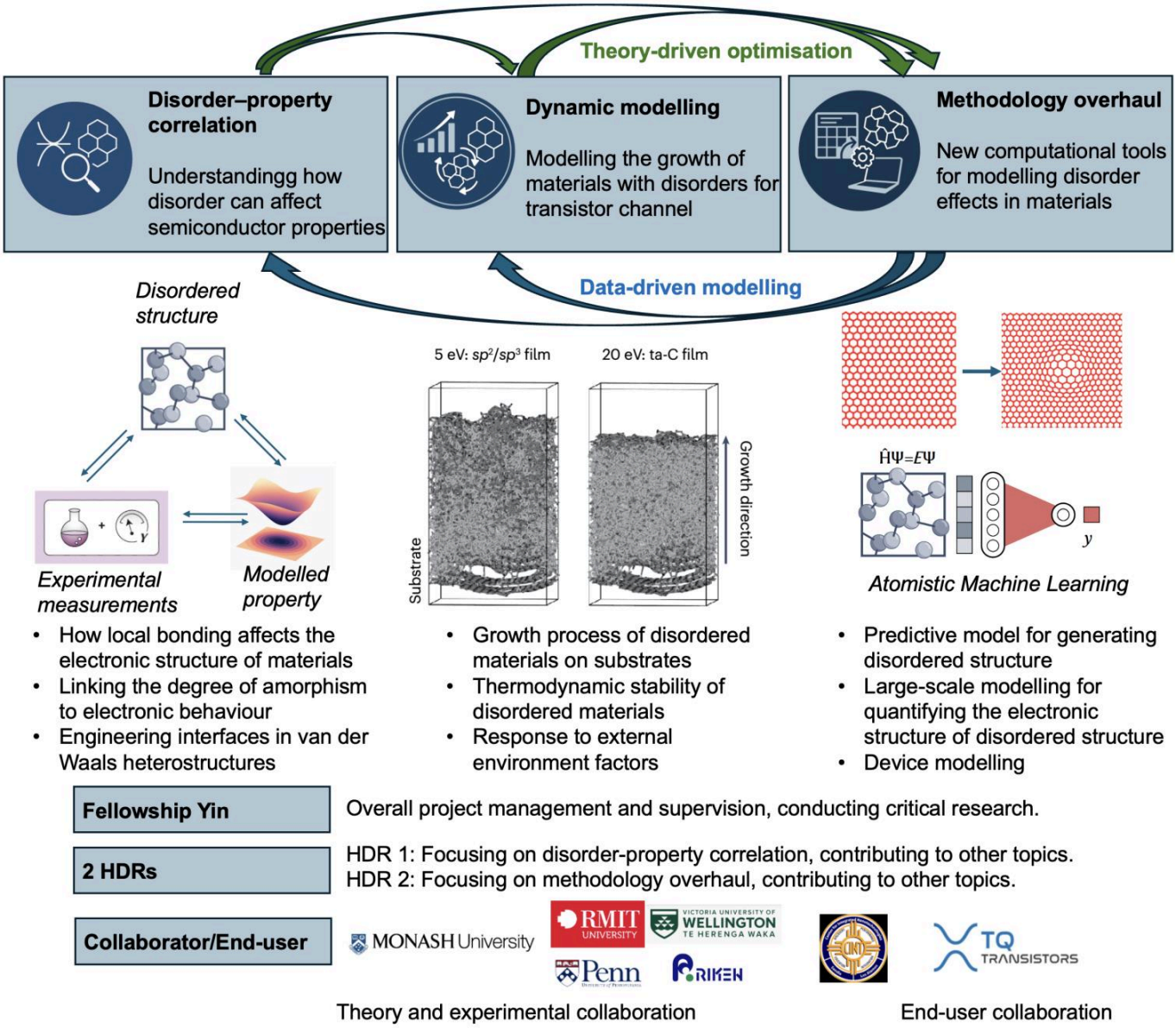

Figure 2. Conceptual framework, project design and team composition of this fellowship.

To fulfil the goal of establishing a new computational paradigm for disorder-oriented materials design and addressing the major research questions in the field, this fellowship will be divided into three distinct but interconnected tasks: **Disorder–Property Correlation (Task 1)**, **Dynamic Modelling (Task 2)**, and **Methodology Overhaul (Task 3)**. The key research philosophies that ensure the successful completion of these tasks are theory-driven optimisation and data-driven modelling. Theory-driven optimisation will provide the physical insights into disorder behaviour—such as identifying favourable disordered configurations—derived from Tasks 1 and 2 as the theoretical foundation for developing computational tools in Task 3. In turn, the outcomes of Task 3 will deliver advanced data-driven modelling methods to analyse the datasets generated from Tasks 1 and 2, uncover hidden correlations, validate theoretical predictions, and identify new design pathways. Together, these two complementary approaches form a closed feedback loop—where theory refines models and data strengthens theory—establishing an iterative, self-consistent workflow that accelerates the discovery and optimisation of disorder-oriented materials.

This fellowship will assemble a strong team to deliver excellence in research, training, and collaboration. Dr Yin will apply his expertise in computational materials science and condensed matter physics to lead critical research across all three tasks, supervise 2 HDR students, and collaborate with global experts in

the field. HDR 1 will focus primarily on Task 1, investigating the correlation between amorphism and electronic transport, and applying these insights to optimise interfaces in transistor structures. HDR 2 will focus primarily on Task 3, using physics knowledge and computational algorithms to overhaul the modelling process for disordered materials. Both students will also contribute to other Tasks by generating datasets and/or assisting in optimising workflows for the disorder-modelling toolkit.

In terms of collaboration, Dr Yin will work closely with world-renowned condensed matter physicist Prof. Michael Fuhrer, amorphous materials expert A/Prof. Julie Karel, and leading computational materials scientist Prof. Nikhil Medhekar at Monash University. He will also maintain and expand collaborations with research groups at RMIT University (RMIT Applied Quantum Technologies), Victoria University of Wellington (New Zealand), University of Pennsylvania (USA), and RIKEN (Japan). Some experimental validation will be in collaboration with the Center for Integrated Nanotechnologies (CINT) at Sandia National Laboratories (USA). The fellowship will further collaborate with TQ Transistors to support research translation and end-user engagement.

In the following, I will briefly outline the key research topics and objectives associated with each task.

Task 1: Disorder–Property Correlation: The aim of this task is to identify the physical principles that govern how disorder influences the electronic and topological properties of materials. Based on my previous research, in materials lacking long-range periodicity, the preservation of short-range crystalline features is crucial for maintaining desirable electronic characteristics (Top10#1, #4, #5, #7). Therefore, the task will begin by investigating the role of local symmetry in disordered systems. Two contrasting scenarios will be examined: a "low-symmetry" hotspot within an otherwise high-symmetry bulk, and a "high-symmetry" hotspot embedded in an amorphous matrix. Building on these cases, the study will address a more fundamental question—how to define the degree of amorphism. This involves determining the boundaries between regions with different levels of structural disorder. Through these investigations, the electronic responses associated with various disordered configurations, obtained from combined DFT and tight-binding (TB) calculations and experimental measurements, will be correlated to establish a general principle for "placing" disorder in materials. Once these rules are formulated, they will be tested by designing interfacial structures at transistor channels, where bulk, surface, and edge defects often coexist. The task will explore both low-disorder and amorphous regimes to identify candidate disordered material systems suitable for transistor applications.

Task 2: Dynamic Modelling: The aim of this task is to understand the dynamic stability and growth mechanisms of disordered materials during synthesis and operation. Rather than immediately conducting full dynamic modelling, which is computationally demanding, the task will first uncover the underlying physics governing disorder dynamics through a more "static" approach (Top10#4, #10). Representative structural snapshots of disordered materials will be constructed, integrating the design principles developed in Task 1 and insights from experimental observations. Environmental factors such as temperature and pressure will be systematically introduced to examine the structural and electronic response of these systems. By linking a series of such snapshots, an initial predictive model will be developed to qualitatively describe the dynamic behaviour of disorder evolution. This model will then guide subsequent dynamic simulations, which will be used to test and refine the theoretical framework. The outcome of this task will be a comprehensive understanding of the growth processes of disordered semiconductor materials and their interactions with substrates and external environments. The dynamic modelling will incorporate quantum-mechanical principles alongside machine learning algorithms to achieve a balance between efficiency and accuracy.

Task 3: Methodology Overhaul: The aim of this task is to develop new computational tools for accurately modelling the properties of disordered materials. Building on my existing quantum materials modelling framework established through the "Bismuth Trilogy" studies (Top10#1, #2, #3), this task will extend those methods to large-scale simulations of disordered and amorphous systems. New theory-driven algorithms will be designed and enhanced using machine learning to create tools for both static and dynamic modelling, directly supporting the investigations in Tasks 1 and 2. The innovation in this task lies in delivering new physics and new algorithms for methodological development. First, I will propose novel physical algorithms capable of quantifying atomic nearest neighbours, coordination environments, and site symmetries—critical parameters for characterising the local structures of amorphous materials. Second, I will bridge the current length-scale gap between atomistic and device-level simulations, establishing a unified and transferable modelling platform that can seamlessly connect quantum-scale calculations with macroscopic performance metrics. The outcome of Task 3 will be a robust computational framework that integrates the physical principles developed in Tasks 1 and 2. This tool will

enable efficient prediction of electronic behaviour in disordered systems and facilitate large-scale device modelling, providing a powerful platform for disorder-oriented materials design.

In summary, these three tasks form a unified framework for disorder-oriented materials design grounded in new physical principles, and the success of the fellowship will revolutionise our understanding of the physics of disorder and transforming the way disordered systems are studied and modelled.

BENEFIT

New and Advanced Knowledge: This fellowship will generate critical and transformative knowledge in materials science by establishing a new design paradigm where atomic disorder is engineered as a functional advantage rather than a limitation. It will deliver a computational and theoretical framework that quantitatively links disorder to electronic, magnetic and transport properties of materials, providing predictive control over material performance. Advanced theory-driven algorithms developed through this project will enable large-scale simulations combined with machine learning that reveal disorder-induced quantum phenomena previously inaccessible to traditional approaches. The resulting knowledge will broaden fundamental understanding of non-crystalline and complex materials, leading to significant advances in emerging technologies such as energy-efficient electronics and quantum computing.

Economic, Commercial, Environmental and Social Benefits: The success of this fellowship will benefit the global semiconductor research and development community by providing essential knowledge for growing disordered materials for electronic device fabrication. It will reaffirm Australia's leading role in pioneering scientific breakthroughs that advance technology and improve human life. The open-source computational tools developed through this fellowship will accelerate the modelling of disordered systems, with the aim of making them a widely adopted and preferred choice within the international research community. The strong collaborative network established through this fellowship spanning universities, research institutes, and end-users will foster continuous knowledge exchange, strengthen Australia's research capabilities, and promote sustained international engagement. Finally, the fellowship will help cultivate a highly skilled workforce in advanced manufacturing and quantum technologies—areas that are vital for maintaining Australia's technological competitiveness in the future.

Although most of the research undertaken in this fellowship is fundamental in nature, its potential economic and commercial impact is unprecedented if the generated knowledge can be integrated into the fabrication of economically viable non-silicon electronic devices. Such an advancement would also deliver significant environmental benefits, bringing society closer to achieving a net-zero future. This outcome would reaffirm the importance of conducting basic research, which may not yield immediate results but will drive long-term technological progress and social benefits.

Lastly, this fellowship will serve as a model for the Australian research community by demonstrating the power of computational modelling in driving real-world technological advancement. At present, Australia is still short of expertise in computational materials science, particularly in methodological design and development. This fellowship will help address that gap by positioning me as an emerging leader in the field, leading to a more diverse, innovative, and internationally competitive research landscape.

MENTORING AND CAPACITY BUILDING

Alignment of Expertise with Project Aims: This fellowship builds directly on my established expertise in computational materials science. Over the past decade, I have advanced the fundamental understanding of topological and spintronic materials and developed scalable computational codes for large-cell simulations of electronic and magnetic structures. This expertise directly supports the project's aim to develop a predictive framework for disorder-oriented materials design. In addition, the strong computational infrastructure at Monash University, combined with its national leadership in nanofabrication and materials characterisation, provides an ideal environment for conducting large-scale modelling and experimental validation.

Advancing National and International Leadership through Collaboration: As outlined in the Project Design, this fellowship will strengthen and expand connections with both domestic and international research institutions. I will first use the collaborations established during my time at the ARC Centre of Excellence in Future Low-Energy Electronic Technologies (FLEET) to form new working groups on disordered materials with researchers from leading Australian alliances such as the Quantum Light, Information, Matter and Electronics (QLIME) group at Monash University and the RMIT Applied Quantum Technologies (RAQT) group. Through these collaborations, I aim to develop joint research projects that will be competitive for future ARC funding opportunities.

Second, I will take the lead in enhancing the Trans-Tasman research partnership in quantum materials by establishing research exchanges with the Robinson Institute at Victoria University of Wellington, which recently received NZ$71 million funding to advance electronic technology development. Strengthening ties with New Zealand will help elevate Oceania's global research leadership in this field.

Finally, I plan to visit leading research groups and laboratories in Japan and the United States to engage with world-class researchers and foster reciprocal exchange programs. These international interactions will provide exposure to diverse research environments and funding opportunities, further developing my leadership and strengthening Australia's presence in the global research community.

Mentoring and Research Training for the Next Generation: The fellowship will foster a vibrant environment for mentoring and capacity building for both me and the HDR students involved. I will supervise two PhD students directly supported through the fellowship and Monash University's research programs. Through regular meetings, tutorials, and shared online resources, students will develop advanced skills in electronic structure theory, high-performance computing, and data-driven modelling. These activities will be closely guided by my supervision philosophy, which encourages research independence, critical thinking, and interdisciplinary learning. This approach ensures that students not only acquire technical expertise but also develop the confidence and creativity needed to lead their own research directions. I believe that students immersed in such an environment will become exceptional researchers and contribute directly to the success of the fellowship. Monash University will also provide extensive professional development opportunities to prepare students for careers beyond their PhD studies. Overall, the fellowship will enhance student training in the field of quantum and strengthen my own leadership and mentoring capabilities, which will be critical for the advancement of my academic career.

COMMUNICATION OF RESULTS

Results from this project will be communicated through journal publications, conferences, and online media.

- **Journal Publications**: I expect to publish around ten papers as leading or corresponding author during the fellowship in prestigious journals in materials science and condensed matter physics, such as *ACS Nano, Physical Review Letters, Science Advances,* and *Nature Communications*. I am also confident that the project will yield discoveries of sufficient significance for top-tier journals such as *Science* and *Nature*, which would help expose this research to a broad international audience.
- **Conferences and Workshops**: I will present my findings at major domestic and international conferences, including the *American Physical Society Global Physics Summit* and the *Materials Research Society Spring and Fall Meetings*. I also intend to take on leadership roles in organising workshops in Australia to foster the growth of the condensed matter research community, with a particular emphasis on advancing the application of computational materials design.
- **Online Media**: I will use social media platforms, short videos, and podcasts to communicate new knowledge generated from this fellowship to the public. Specialised content will be created for younger audiences to promote awareness of materials science and computational modelling within school education. In addition to these outreach activities, all data and algorithms developed in this project will be made publicly available on GitHub to further support the advancement of the field.

REFERENCES

Citation "Top10#" refers to the 10 Career-Best Research Outputs listed in Section B11 of this fellowship application. Sources for Figure 1 are labelled on the Figure. Source for subfigures in Figure 2: Y. Liu et al., *Nat. Rev. Mater.* 2025, 10, 228.