Australian Research Council

Future Fellowships 2027

Consolidated application working draft

Application information	
Project ID	Not assigned - FT27 draft
First investigator	Dr Yuefeng Yin
Administering organisation	Monash University
Application title	Beyond Order: Disorder-Oriented Design of Quantum Materials
Previous application reference	FT260101712 - submitted 5 November 2025
Draft updated	9 September 2026

DRAFT - NOT FOR SUBMISSION

This local review copy follows the A-F order of the supplied RMS application. It contains all information held in the working data, including the five supporting documents. It is not an RMS export. Historical responses and institutional support require confirmation for FT27.

Page and field limits are inherited from FT26 and must be checked against the FT27 instructions. The source PDF does not display B2; no B2 response is invented. Certification must be completed by the authorised institution in RMS.

- Part A - Administrative Summary
- Part B - Participant Details including ROPE
- Part C - Project Description and Letter of Support
- Part D - Project Cost
- Part E - Classifications and Statistical Information
- Part F - Project Eligibility
- Review notes and certification status

Part A - Administrative Summary

A1. Application Title

FT26 reference: up to 75 characters; approximately 10 words.

Beyond Order: Disorder-Oriented Design of Quantum Materials

A2. Person Participant Summary

Name	Participant type	Current organisation
Dr Yuefeng Yin	Future Fellowship	Monash University

A3. Organisation Participant Summary

Name	Participant type
Monash University	Administering Organisation

A4. Application Summary

FT26 reference: up to 750 characters; approximately 100 words.

This project aims to develop new strategies for designing advanced materials in which structural disorder is viewed as a source of useful functionality rather than a detrimental effect. Using state-of-the-art computational modelling approaches, the fellowship will uncover new classes of disordered materials with tailored electronic and quantum properties for next-generation chips and computing devices. Expected outcomes include durable, low- energy and fabrication-friendly materials compatible with existing semiconductor platforms. The project will place Australia as a global leader in semiconductor innovation and accelerate the shift toward a more connected, energy-efficient and sustainable technological future.

A5. National Interest Test Statement

FT26 reference: up to 1500 characters; approximately 200 words.

The energy demand of modern technologies is growing far faster than the energy efficiency of the electronic devices that sustain them. To overcome this imbalance, new materials are urgently needed to reduce power consumption without compromising performance. While current materials design approaches are highly effective for studying crystalline materials, they remain limited in exploiting the advantages of atomic disorder, which is known to influence conductivity, stability, and durability but cannot yet be controlled or optimized in a predictable way. This project will transform that challenge into an opportunity by developing a new computational framework to model and harness disorder as a functional design feature.

By identifying materials that are more durable, energy-efficient, and easier to manufacture, this fellowship will help Australia lead the development of next-generation semiconductors and quantum devices that support sustainable and low-energy computing. The advanced algorithms developed from the fellowship will enhance Australia's digital materials design capability and strengthen collaboration between universities, research institutes, and industry. The fellowship will train skilled researchers in data-driven modelling and semiconductor science, aligning with national priorities in advanced manufacturing and quantum technologies, and positioning Australia as a global leader in innovative, energy-efficient materials for future information technologies.

Part B - Participant Details including ROPE

B1. Personal Details

Item	Response
Participation type	Future Fellowship
Title	Dr
First name	Yuefeng
Middle name	Not recorded
Family name	Yin

B3. Qualifications

Conferral date	AQF level	Title	Discipline	Organisation	Country
08/03/2016	Doctoral Degree	Doctor of Philosophy	Materials Science and Engineering	Monash University	Australia
20/11/2011	Bachelor Honours Degree, Graduate Certificate, Graduate Diploma	Bachelor Degree with First Class Honours	Materials Engineering	Monash University	Australia

B4. Research Load - non-ARC Grants and Research

No entries recorded in the FT26 baseline.

> Historical empty table; refresh the required reporting period and current funding for FT27.

B5. Current and Previous Appointments

Description	Department	Contract type	Employment type	Start date	End date	Organisation
Research Fellow	Department of Materials Science and Engineering	Contract	Full Time	01/10/2024		Monash University
Research Fellow	Department of Materials Science and Engineering	Contract	Full Time	13/04/2019	01/08/2024	Monash University
Research Fellow	School of Physics and Astronomy	Contract	Full Time	01/04/2017	12/04/2019	Monash University

B6. Career Interruptions

Yes

Researcher Dr Yuefeng Yin has reported a career interruption of 1 year since 2016.

B7. Career Narrative

FT26 reference: up to 565 characters; approximately 75 words.

I have worked as a computational materials scientist at Monash University, with over 90% of my time devoted to research on computational materials design, electronic/spintronic structure modelling and algorithm development, and the remainder on teaching computational modelling and condensed matter physics. My research opportunities have been consistently supported by the ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET), the National Computational Infrastructure (NCI), and domestic/international industry collaborations.

Research impact and contributions to the field

My research connects first-principles theory, electronic and spintronic structure modelling, and device-scale prediction to understand and design quantum and low-dimensional materials. Three contributions establish the scientific and translational foundations of this Fellowship.

Electronic response to disorder and amorphous structure

Achievement and impact: My studies of defective, amorphous and partially ordered materials show how controlled disorder can produce electronic performance comparable to, or better than, crystalline counterparts. Corresponding-authored papers with experimental collaborators demonstrate the tuning of quantum materials' electronic properties. This work has established collaborations with the MacDiarmid Institute in New Zealand and research groups in Japan and China. FLEET provided $10,000 in dedicated travel support for my MacDiarmid collaboration. Following a 2024 Memorandum of Understanding, an R&D project on large-scale disorder-enhanced thin-film growth, co-led by me, was finalised with Jiangxi Copper (https://bit.ly/4oF52AJ).

Relevance: These findings provide the physical basis and experimental links for treating disorder as a controllable design variable. The Fellowship will extend these insights into predictive relationships between atomic disorder and useful electronic behaviour.

A multiscale quantum materials modelling framework

Achievement and impact: I developed a modelling framework linking atomistic first-principles simulations to device-scale calculations, addressing inconsistencies that arise when modelling scales are treated independently. Its application in my three "Bismuth Trilogy" papers reveals topologically nontrivial transport phenomena in ultrathin bismuth films and connects atomic interactions to macroscopic electronic behaviour. Development has been supported by competitive allocations of 3.5 million NCI service units since 2023 (approximately $140,000) and 1 million Pawsey service units since 2025 (approximately $20,000).

Relevance: This framework is the methodological foundation for integrating atomic-scale disorder into larger-scale predictions. Generalising it will connect the Fellowship's theoretical discoveries with device performance and semiconductor applications.

Bilayer structures for transistor channels

Achievement and impact: Since 2024, I have contributed basic and applied research to an R&D program with Australian start-up TQ Transistors to design a novel transistor channel. The collaboration identified promising channel materials and refined fabrication methods. In 2025, the team filed a patent application with me as lead inventor (Application No. US63/848,059), and I finalised a research paper describing the discoveries. The work provides knowledge for developing low-energy transistor materials and their large-scale production.

Relevance: This contribution demonstrates my ability to translate computational materials research into semiconductor development and work with researchers, industry and end users. These capabilities support the Fellowship's pathway from theoretical prediction to experimental fabrication and research translation.

B9. Mentoring and Leadership

FT26 reference: up to 750 characters; approximately 100 words.

I have co-supervised 2 PhD students (1 graduated) and mentored 6 PhD students (4 graduated), 2 Master's students and 6 undergraduates. This work has resulted in 6 published journal papers with me as corresponding author (plus 2 under review), and 4 oral conference presentations, including at the APS March Meeting, with me listed as supervisor. My supervision develops research independence, interdisciplinary skills and critical thinking, encouraging students to pursue original research. I also lead research training through practical materials, hands-on notes and code examples.

> [FT27 TODO] Confirm supervision, publication and presentation counts; condensed from FT26 evidence.

B10. Research Output Context

FT26 reference: up to 1500 characters; approximately 200 words.

In computational materials science and condensed matter physics, peer-reviewed journal articles are the main measure of research quality and impact. My work integrates first-principles theory and data-driven modelling to address fundamental questions in quantum and disordered materials. To date, I have published 40 peer-reviewed journal articles, with an h-index of 17 and over 1,000 citations—consistent with field norms, as computational condensed matter research generally receives fewer citations than experimental or applied STEM areas.

My publications demonstrate systematic investigation of emerging topics in materials science. For example, I have published five papers on the electronic and spintronic structures of two-dimensional quantum materials bismuth allotropes, proposing new physical models and revealing novel quantum phenomena, with results published in Mater. Today Phys., Phys. Rev. B, and New J. Phys. Another major focus involves tuning the electronic properties of magnetic topological materials through controlled disorder, with results published in ACS Nano, Matter, Nano Lett., and npj Quantum Mater.

I am frequently the corresponding or lead theoretical author for model design and analysis. My interdisciplinary collaborations have led to high-impact papers in Nat. Commun., Adv. Mater., and Adv. Funct. Mater. Overall, my research outputs demonstrate my originality, leadership, and research excellence in computational materials.

> [FT27 TODO] update publication/citation/h-index counts to current figures before submission.

B11. Ten Career-Best Academic Research Outputs

> [FT27 TODO] review for any papers published since Nov 2025 that should displace a weaker entry; recompute h-index/citations in B10 to match.

[1] * Yin, Yuefeng, Wang, Chutian, Fuhrer, Michael S. & Medhekar, Nikhil V. 2023, 'Extracting unconventional spin texture in two dimensional topological crystalline insulator bismuthene via tuning bulk-edge interactions', Materials Today Physics, vol. 36, pp. 101168, doi:10.1016/j.mtphys.2023.101168 (Refereed Journal Article)

Research output annotation: Proposes a novel design principle for nanoelectronics via bulk-boundary disorder effects; part of the "Bismuth Trilogy" and foundation of a patent.

[2] * Wang, Chutian, Yin, Yuefeng, Huynh, Thanh Tung, Fuhrer, Michael S. & Medhekar, Nikhil V. 2025, 'Edge State Stabilization and Control in 2D Topological Crystalline Insulators', Materials Today Physics, pp. 101897, doi:10.1016/j.mtphys.2025.101897 (Refereed Journal Article)

Research output annotation: Corresponding paper proposing a setup to stabilise topological phases in 2D bismuth using substrate, pressure and field; part of "Bismuth Trilogy."

[3] * Li, Qile, Smith, Jackson S, Yin, Yuefeng, Wang, Chutian, Klymenko, Mykhailo V, Cole, Jared H & Medhekar, Nikhil V 2021, 'Localized Wannier function based tight-binding models for two-dimensional allotropes of bismuth', New Journal of Physics, vol. 23, no. 6, pp. 063042, doi:10.1088/1367-2630/ac04c9 (Refereed Journal Article)

Research output annotation: Corresponding paper presenting an efficient method to derive effective models for quantum materials with DFT accuracy; part of the "Bismuth Trilogy."

[4] * Zhao, Weiyao, Zhang, Yao, Yin, Yuefeng, Xing, Kaijian, Zhou, Shengqiang, Bake, Abdulhakim, Akhgar, Golrokh, Cortie, David, Chen, Lei, Wang, Xiaolin, Rule, Kirrily C., Medkehar, Nikhil V., Granville, Simon & Karel, Julie 2025, 'Giant berry curvature in amorphous ferromagnet Co2MnGa', Matter, vol. 8, no. 3, pp. 101988, doi:10.1016/j.matt.2025.101988 (Refereed Journal Article)

Research output annotation: Co-first-authored paper reporting the first observation of large anomalous Hall conductivity in an amorphous topological compound (Co2MnGa).

[5] * Zhang, Yao, Yin, Yuefeng, Dubuis, Guy, Butler, Tane, Medhekar, Nikhil V. & Granville, Simon 2021, 'Berry curvature origin of the thickness-dependent anomalous Hall effect in a ferromagnetic Weyl semimetal', npj Quantum Materials, vol. 6, no. 1, doi:10.1038/s41535-021-00315-8 (Refereed Journal Article)

Research output annotation: Co-first-authored paper reporting the effect of film thickness on the electronic structure of Co_2MnGa.

[6] * Wang, Jinlong, Zhang, Yao, Hu, Junfeng, Song, He, Sun, Xiaozhen, Meng, Xiangrui, Xu, Ziyue, Yin, Yuefeng, Yang, Tianyu, Sheng, Lutong, Chen, Jilei, Liu, Song, Li, Peng, Gao, Peng, Medhekar, Nikhil V., Yu, Dapeng, Granville, Simon & Yu, Haiming 2025, 'Band Structure Engineering to Optimize Spin-Wave Propagation in Weyl ferromagnet Co2MnGa1-xGex', Advanced Materials, doi:10.1002/adma.202505704 (Refereed Journal Article)

Research output annotation: Collaboration with experiments reporting how atomic disorders (alloying) influences the electronic structure of Co_2MnGa.

[7] * Yin, Yuefeng, Fuhrer, Michael S. & Medhekar, Nikhil V. 2019, 'Selective control of surface spin current in topological pyrite-type OsX2 (X = Se, Te) crystals', npj Quantum Materials, vol. 4, no. 1, doi:10.1038/s41535-019-0186-8 (Refereed Journal Article)

Research output annotation: First theoretical identification of this Os-based compound as topological; demonstrates anisotropic surface spin current in a non-magnetic material.

[8] * Xing, Kaijian, McEwen, Daniel, Yin, Yuefeng, Zhao, Weiyao, Bake, Abdulhakim, Cortie, David, Liu, Jingying, Vu, Thi-Hai-Yen, Chen, Yi-Hsun, Hone, James, Stacey, Alastair, Edmonds, Mark T., Medhekar, Nikhil V., Watanabe, Kenji, Taniguchi, Takashi, Ou, Qingdong, Qi, Dong-Chen & Fuhrer, Michael S. 2025, 'Pick-and-Place Transfer of Arbitrary-Metal Electrodes for van der Waals Device Fabrication', ACS Nano, vol. 19, no. 3, pp. 3579-3588, doi:10.1021/acsnano.4c13592 (Refereed Journal Article)

Research output annotation: Co-first-authored paper showing a universal method for transferring electrodes, enabling scalable and flexible van der Waals device fabrication.

[9] * Tang, Lingyun, Mao, Zhongquan, Wang, Chutian, Fu, Qi, Wang, Chen, Zhang, Yichi, Shen, Jingyi, Yin, Yuefeng, Shen, Bin, Tan, Dayong, Li, Qian, Wang, Yonggang, Medhekar, Nikhil V., Wu, Jie, Yuan, Huiqiu, Li, Yanchun, Fuhrer, Michael S. & Zheng, Changxi 2023, 'Giant piezoresistivity in a van der Waals material induced by intralayer atomic motions', Nature Communications, vol. 14, no. 1, doi:10.1038/s41467-023-37239-9 (Refereed Journal Article)

Research output annotation: Reveals giant piezoresistivity in a van der Waals material driven by intralayer atomic motions, advancing strain-engineered quantum device design.

[10] * Yin, Yuefeng, Cervenka, Jiri & Medhekar, Nikhil V. 2017, 'Molecular Dipole-Driven Electronic Structure Modifications of DNA/RNA Nucleobases on Graphene', The Journal of Physical Chemistry Letters, vol. 8, no. 13, pp. 3087-3094, doi:10.1021/acs.jpclett.7b01283 (Refereed Journal Article)

Research output annotation: Proposes a theory on how molecular dipoles affect the interaction between DNA/RNA and graphene, advancing the application of graphene in biosensing.

B12. Currently Held ARC Projects

No entries shown in the FT26 application.

> [FT27 TODO] Refresh from the participant's current RMS record.

B13. Relevant Qualification

Conferral date	AQF level	Title	Discipline	Organisation	Country
08/03/2016	Doctoral Degree	Doctor of Philosophy	Materials Science and Engineering	Monash University	Australia

B14. Eligibility Period Extension Granted

No

> Historical FT26 answer; confirm against FT27 eligibility dates and current certification.

B15. Career Interruption Category Claimed

Not completed / blank in the working data.

B16. Total Extension Period Claimed

Not completed / blank in the working data.

B17. Professional Equivalent to a PhD

Yes

> [FT27 TODO] The source PDF page 11 records Yes even though B13 lists a PhD. Confirm this response with the Research Office; retained faithfully here.

B18. Current Academic Level

Level B

Part C - Project Description

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.

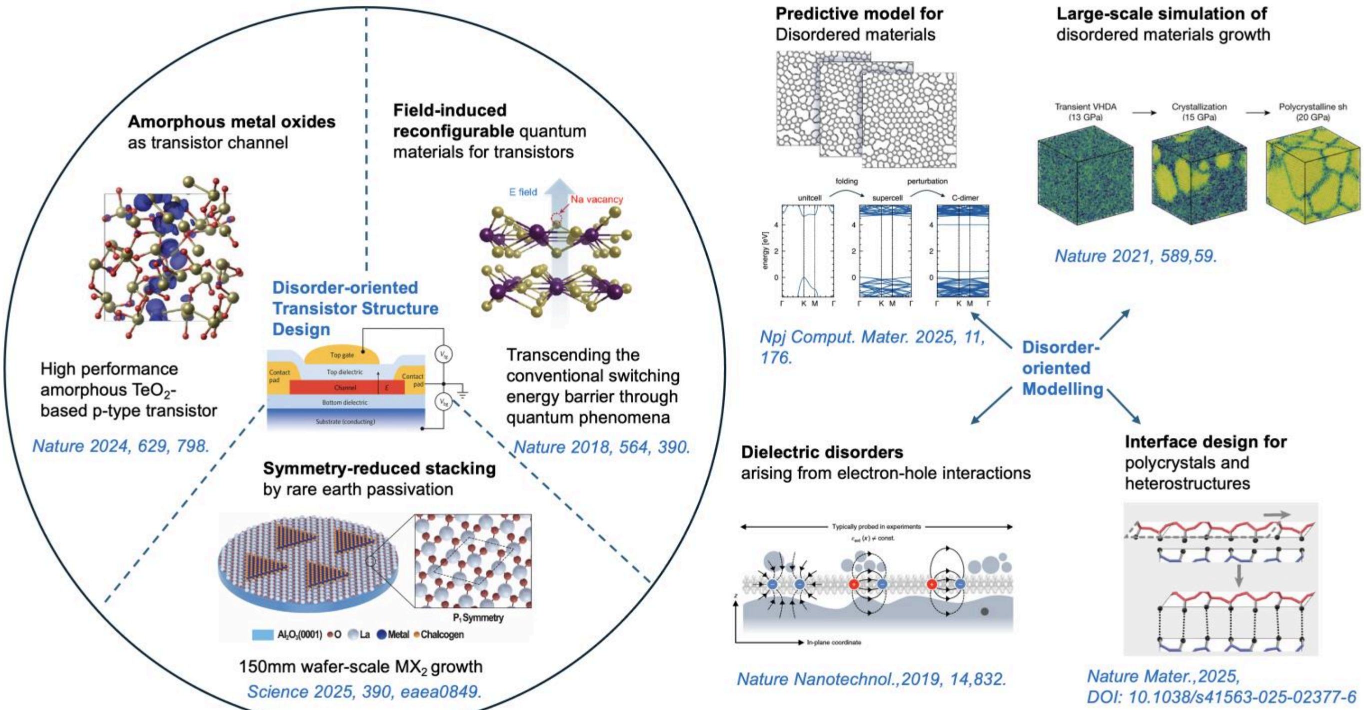

Figure 1. (Left) Recent significant advances in transistor structure design that incorporate disorders as key elements. (Right) Key topics for disorder-oriented modelling.

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

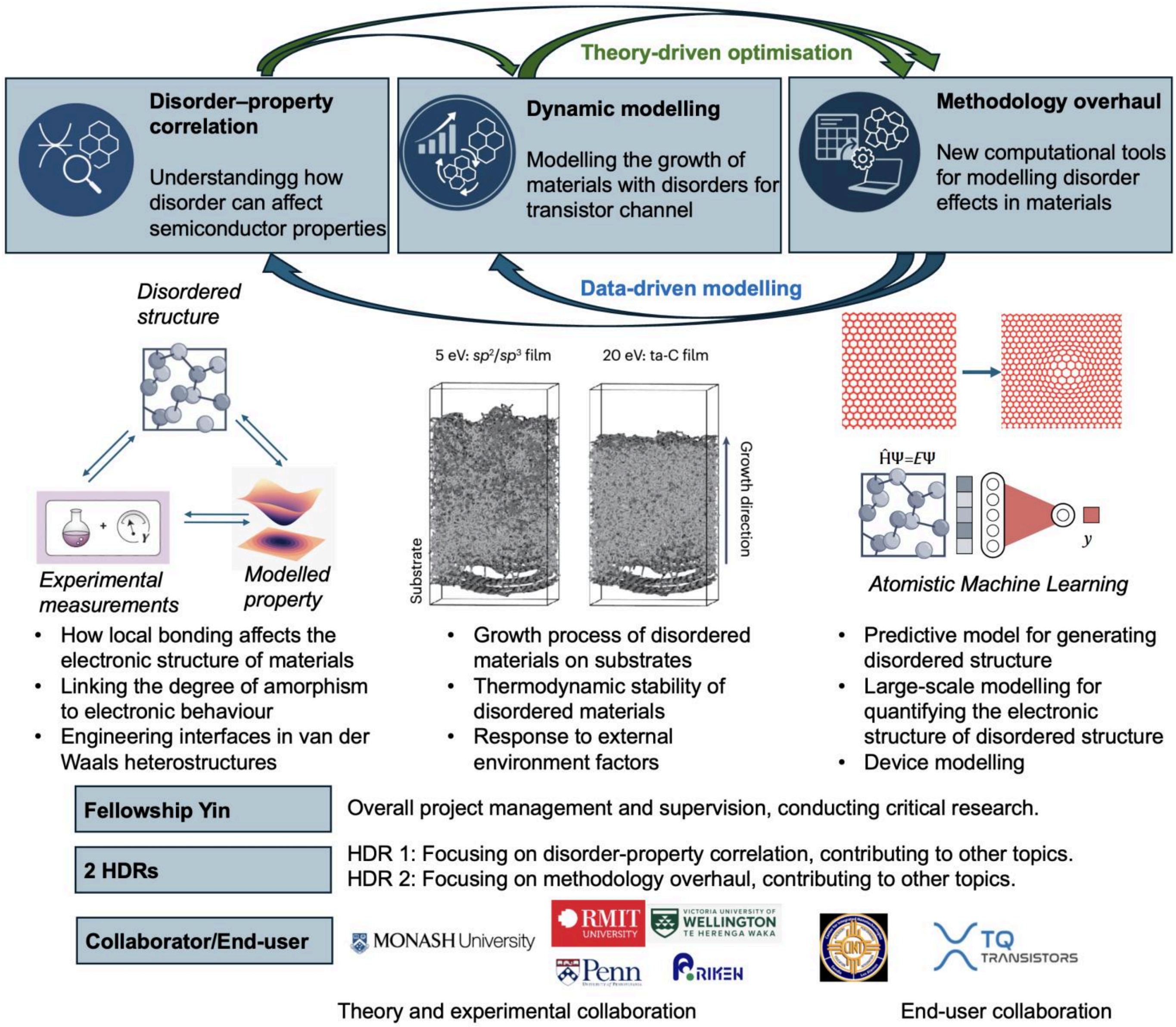

Figure 2. Conceptual framework, project design and team composition of this fellowship.

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.

C2 — Administering Organisation Letter of Support

30 October 2025

Professor Ute Roessner
Chief Executive Officer
Australian Research Council
GPO Box 2702
CANBERRA ACT 2601

Dear Professor Roessner,

Monash University strongly supports the Future Fellowship application of Dr Yuefeng Yin in the Department of Materials Science and Engineering (DMSE). Dr Yin is an outstanding mid-career computational materials scientist whose research expands materials science, condensed matter physics, and data-driven modelling. Dr Yin has established strong expertise and a reputation for innovation in theoretical and computational design of quantum materials, with his research published in leading international journals such as ACS Nano, Materials Today Physics, Nano Letters, Matter, and npj Quantum Materials. He has developed unique proficiency in multiscale modelling and automated simulation workflows, supported by major computational grants from the National Computational Infrastructure (NCI) and the Pawsey Supercomputing Centre. As a core member of the ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET), Dr Yin plays a central role in bridging theory and experiment for quantum and topological materials. His interdisciplinary collaborations with physicists, materials engineers, and industry partners have positioned him as an emerging leader in computational quantum materials research in Australia. He has also played pivotal roles in research translation and commercialisation through his recent collaboration with the Australian start-up TQ Transistors, developing next-generation transistor architectures, which attracts significant investment interests from domestic and international sources.

Dr Yin's Future Fellowship proposal aims to transform *disorder*—traditionally viewed as a limitation—into a functional design element for next-generation semiconductor and quantum technologies. The project will establish a predictive, data-driven computational framework to identify low-energy, fabrication-ready materials that outperform current technology, contributing directly to the global search for alternatives to the limit-reaching silicon chip. The expected outcomes will generate new fundamental knowledge of disordered materials, deliver advanced modelling tools for materials discovery, and strengthen Australia's strategic priorities in advanced manufacturing, critical materials, quantum technology, and the net-zero transition. The Fellowship will consolidate Dr Yin's leadership in computational design and accelerate the nation's capability in developing sustainable, low-energy electronics while expanding Australia's skilled research workforce in quantum technologies.

Alignment with Monash University Research Strengths

Monash University is internationally recognised for research excellence and impact. The University's performance in the latest Excellence in Research for Australia (ERA) evaluation confirmed Materials Engineering as a top-ranked discipline (ERA 5 – well above world standard). The Materials Science research at Monash is consistently ranked among the world's leading institutions—29th globally (QS, 2025)—and is home to several eminent researchers, including Professor Michael Fuhrer, a world-renowned expert in semiconductor materials and a long-term collaborator of Dr Yin. Dr Yin also works closely with Professor Nikhil Medhekar, a leading figure in the Australian computational modelling community, and Associate Professor Julie Karel, an emerging leader in experimental condensed matter.

Monash provides a unique research ecosystem for the success of this Fellowship. The ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET), hosted at Monash, has left a strong foundation for both fundamental and applied research into next-generation quantum and low-energy devices within the Department of Materials Science and Engineering. This environment provides Dr Yin with unrivalled access, among Australian universities, to high-impact internal collaborations across theory and experiment. In addition, Monash's strategic alliance with NCI and the newly built, Australia-first AI supercomputer MAVERIC ensures that Dr Yin will have exceptional computational capability and technical support to deliver on the project's objectives.

The aims of Dr Yin's project align closely with the Faculty of Engineering's strategic plans to conduct mission-oriented, interdisciplinary research that addresses critical global challenges and fosters partnerships for impactful research outcomes. The Fellowship also complements the Department's initiative to strengthen a Quantum Materials and Technology research and teaching stream, responding to growing international interest in quantum technologies. In return, Dr Yin's expertise in semiconductor materials and multiscale modelling will broaden Monash's research portfolio, strengthening interdisciplinary links between materials science, physics, and data science. This mutually reinforcing partnership will consolidate Monash's position at the forefront of computational materials discovery while advancing Dr Yin's development as a world-class researcher in semiconductor innovation and a leading advocate for Australia's transition to a net-zero future.

Research Environment

Monash University provides a rich and collaborative research environment that will strongly support Dr Yin's Future Fellowship and career development. He will draw on the expertise and infrastructure of the Monash eResearch and the Monash Data Futures Institute, which offer world-class high-performance computing, data management, and AI capabilities essential for his computational and data-driven materials design. The DMSE provides advanced facilities and technical expertise for characterisation and validation of complex materials systems proposed in Dr Yin's project. Research development support through Monash Innovation and the Faculty Research Office will assist in grant preparation, interdisciplinary collaborations, and industry engagement, including partnerships with end-users. In addition, Monash's researcher development programs—covering mentoring, leadership, and networking—will further enhance Dr Yin's professional growth. Dr Yin will make invaluable contribution to the Monash research ecosystem by mentoring students, leading interdisciplinary collaborations, and advancing Australia's capabilities in computational materials discovery and critical technologies.

Direct Support for the Research Proposal

The Future Fellowship program at Monash University offers individually tailored professional development in research leadership, impact planning, and interdisciplinary engagement to strengthen the capabilities of our emerging research leaders. The Faculty of Engineering will ensure that Dr Yin has access to all key facilities required to successfully carry out the proposed research, including high-performance computing and data analysis infrastructure. Additionally, the Faculty will provide an HDR stipend to support the project's PhD student. The DMSE will cover the salary/stipend gap for Dr Yin and the PhD student. An academic mentoring committee, comprising a research mentor, a university mentor, and an industry mentor, will provide continuous guidance to support Dr Yin's professional growth and research leadership. These commitments will ensure that Dr Yin's Fellowship achieves its goals and contributes to the long-term advancement of computational and quantum materials research at Monash and in Australia.

Integration into Monash Research Activities

At the end of the Fellowship program, it is expected that Dr Yin will build strong international reputation as an expert in computational and quantum materials design. He will continue to play a key role within DMSE at Monash University, fostering interdisciplinary collaborations and contributing to competitive research initiatives in quantum technologies and advanced manufacturing. Monash University strongly supports Dr Yin's Future Fellowship application and is confident that, upon its completion, he will be well positioned to continue his career as a leading researcher at Monash, driving internationally recognised programs in computational materials discovery and strengthening Australia's capability in low-energy electronic technologies.

Part D - Project Cost

D1. Proposed Budget

[FT27 TODO] These are the verbatim FT26 figures (commencing 2026, so effectively 2026-2029). For FT27 (commencing 2027), re-index: (1) shift the four years to 2027-2030, (2) update Dr Yin's Level B salary point and on-costs to the rate current at FT27 lodgement, (3) update the ARC HDR stipend rate for the relevant year, (4) re-check conference years/venues in the travel plan (D2) still make sense for a 2027 start, (5) recompute all year and grand totals once rates are updated.

Name	Role	Schedule
Dr Yuefeng Yin	Future Fellowship	Level 1 from year 1 annually for 4 years
HDR	Higher Degree by Research stipend	Level 1 from year 1 annually for 4 years

Year 1

Description	ARC cash	Monash cash
Dr Yuefeng Yin (Future Fellowship)	$191,726	$3,126
HDR (Higher Degree by Research stipend)	$33,533	$3,612
HDR (Higher Degree by Research stipend) - Monash Contribution	-	$37,145
Personnel subtotal	$225,259	$43,883
Travel	$2,500	-
Equipment	$22,985	-
Other	$0	-
Year total	$250,744	$43,883

Year 2

Description	ARC cash	Monash cash
Dr Yuefeng Yin (Future Fellowship)	$191,726	$3,352
HDR (Higher Degree by Research stipend)	$33,533	$3,612
HDR (Higher Degree by Research stipend) - Monash Contribution	-	$37,145
Personnel subtotal	$225,259	$44,109
Travel	$15,375	-
Equipment	$0	-
Other	$11,000	-
Year total	$251,634	$44,109

Year 3

Description	ARC cash	Monash cash
Dr Yuefeng Yin (Future Fellowship)	$191,726	$3,591
HDR (Higher Degree by Research stipend)	$33,533	$3,612
HDR (Higher Degree by Research stipend) - Monash Contribution	-	$37,145
Personnel subtotal	$225,259	$44,348
Travel	$15,440	-
Equipment	$0	-
Other	$11,000	-
Year total	$251,699	$44,348

Year 4

Description	ARC cash	Monash cash
Dr Yuefeng Yin (Future Fellowship)	$191,726	$13,346
HDR (Higher Degree by Research stipend)	$33,533	$3,612
HDR (Higher Degree by Research stipend) - Monash Contribution	-	$18,573
Personnel subtotal	$225,259	$35,531
Travel	$14,600	-
Equipment	$0	-
Other	$11,000	-
Year total	$250,859	$35,531

Four-year total	Amount
ARC requested	$1,004,936
Monash contribution	$167,871

D2 — Justification of Funding Requested from the ARC

Personnel

Dr Yuefeng Yin (Future Fellowship)

Dr Yin is appointed at Academic Level B, Step 5 at 1.0 FTE + 30% on costs for the four years of the fellowship.

HDR (Higher Degree by Research stipend)

Funding of one Postgraduate Stipend ($33,533 p.a.) is sought through the ARC for a period of 4 years.

Travel

Total Travel

Year 1: Dr Yin will attend the Australian Institute of Physics (AIP) Congress to present his research and engage with both domestic and international members of the physics community. Participation in this conference will strengthen Dr Yin's leadership within Australia's materials physics community, which is essential for advancing the goals of this fellowship.

Cost estimation: $1,000 (registration) + $300 (flight) + $200 (other transportation) + $700 (accommodation) + $300 (food and other incidentals) = $2,500 in total for Dr Yin to attend the 5-day congress.

Year 2: Dr Yin and two HDR students will attend the APS Global Physics Summit in the United States to present research outcomes from the fellowship and engage with the international physics community. Participation in this conference is vital for increasing the visibility of the fellowship's work, fostering new collaborations with leading researchers, and supporting the professional development of Dr Yin and the two HDR students.

Cost estimation: $1,400 (registration) + $6,000 (flight) + $600 (other transportation) + $3,000 (accommodation) + $1,800 (food and other incidentals) = $12,800 in total for Dr Yin and two HDRs to attend the 5-day summit.

Dr Yin will travel to Robinson Institute at Victoria University of Wellington to present his research and interact with fellow researchers to strengthen the Trans-Tasman research collaboration on research on quantum materials, which fulfill this fellowship's vision to advance the international leadership in this field.

Cost estimation: $800 (flight) + $200 (other transportation) + $875 (accommodation) + $700 (food and other incidentals) = $2,575 in total for Dr Yin to undertake a one-week visit.

Year 3: Dr Yin and two HDR students will attend the MRS Spring Meeting in the United States to present research outcomes from the fellowship and engage with the international physics community. Participation in this conference is vital for increasing the visibility of the fellowship's work, fostering new collaborations with leading researchers, and supporting the professional development of Dr Yin and the two HDR students.

Cost estimation: $1,400 (registration) + $6,000 (flight) + $600 (other transportation) + $2,400 (accommodation) + $1,440 (food and other incidentals) = $11,840 in total for Dr Yin and two HDRs to attend the 4-day meeting.

Dr Yin will travel to the Institute of Physical and Chemical Research (RIKEN) in Japan for a strategic visit to present his research and collaborate with leading researchers in the study of the electronic structure of amorphous materials. This visit is essential for the success of the fellowship and for strengthening international leadership in this field.

Cost estimation: $2,000 (flight) + $200 (other transportation) + $700 (accommodation) + $700 (food and other incidentals) = $3,600 in total for Dr Yin to undertake a one-week visit.

Year 4: Dr Yin and two HDR students will travel to the University of New South Wales (UNSW) to attend the Gordon Godfrey Workshop on Spins, Topology, and Strong Electron Correlations, where they will present the research outcome from this fellowship and engage with both Australian and international condensed matter physics community. Participation in this workshop is essential for strengthening Dr Yin's leadership in the field of computational materials science and critical for the training of two HDR students.

Cost estimation: $900 (flight) + $600 (other transportation) + $3,000 (accommodation) + $1,800 (food and other incidentals) = $6,300 in total for Dr Yin and two HDRs to attend the 5-day workshop.

Dr Yin will travel to Sandia National Laboratories and the University of Pennsylvania in the United States for a strategic visit to present his research and explore experimental collaborations on the nanofabrication of disordered materials. This initiative is expected to involve joint experimental work with Prof. Michael Fuhrer and A/Prof. Julie Karel at Monash University. During the U.S. visit, Dr Yin will also engage with end-user groups in the United States through the support of TQ Transistors' U.S. subsidiary to promote the potential research translation of the fellowship's outcomes. This visit will be critical to achieving the goals of the fellowship and will play an important role in Dr Yin's professional development.

Cost estimation: $3,000 (flight) + $500 (other transportation) + $2,800 (accommodation) + $2,000 (food and other incidentals) = $8,300 in total for Dr Yin to undertake a two-week visit.

The total cost for the travel for this fellowship requested from ARC is $2,500 (Year 1) + $15,375 (Year 2) + $15,440 (Year 3) + $14,600 (Year 4) = $47,915.

Equipment

Total equipment

Year 1: A software licence for conducting first-principles calculations is essential. An academic VASP licence will be purchased to support the establishment of Dr Yin's research group and will be shared with two HDR students. The VASP license will need to be used for the period of the fellowship (four years). The cost of a new VASP licence is estimated at $8,000.

A high-performance mobile workstation is necessary for conducting modelling and data analysis for the fellowship of computational nature. Mobile workstation should be able to compile and run complex programs, conduct large-scale visualisations and carry out AI/machine learning tasks, which are all essential functions to fulfill the objective set in the fellowship's tasks. Three workstations will be purchased for Dr Yin and two HDR students. These mobile workstations will need to be used for the period of the fellowship (four years). An excellent candidate will be Apple MacBook Pro 14-inch M4 MAX/64 GB RAM/1TB SSD, cost at $4,995 (Apple Educational pricing). Then the total cost will be estimated as $14,985.

The total cost for the equipment for this fellowship requested from ARC is $8,000 + $14,985 = $22,985 (Year 1 only).

Other

Total other expense

Year 2: Article Processing Charges (APC) are required to publish research outcomes from the fellowship in high-impact open-access journals such as Nature Communications and Science Advances. The APC is estimated at $11,000 per article. Funding for one publication is allocated for this year.

Year 3: APC funding is requested for one publication at $11,000.

Year 4: APC funding is requested for one publication at $11,000.

The total cost for Other for this fellowship requested from ARC is $11,000 (Year 2) + $11,000 (Year 3) + $11,000 (Year 4) = $33,000.

D3 — Details of Non-ARC Contributions

Personnel

Dr Yuefeng Yin (Future Fellowship)

The salary difference between Future Fellowship salary and Level B of Monash salary will be covered by Department of Materials Science and Engineering (DMSE), Monash University for the period of the fellowship.

The total cash contribution from DMSE, Monash University for covering this difference is $3,126 (Year 1) + $3,352 (Year 2) + $3,591 (Year 3) + $13,346 (Year 4) = $23,415.

HDR (Higher Degree by Research stipend)

The stipend difference between ARC HDR stipend and Monash PhD scholarship will be covered by Department of Materials Science and Engineering (DMSE), Monash University for the period of the fellowship.

The total cash contribution from DMSE, Monash University for covering this difference is $3,612 (Year 1) + $3,612 (Year 2) + $3,612 (Year 3) + $3,612 (Year 4) = $14,448.

HDR (Higher Degree by Research stipend) – Monash Contribution

Funding of an additional Postgraduate Stipend ($37,145 p.a.) is funded through Faculty of Engineering, Monash University for a period of 3.5 years.

Part E - Classifications and Other Statistical Information

E1. Australian Government Priority Areas

- National Quantum Strategy, 2023.
- Australia Government's Critical Technologies Statement, 2023.
- Australia's National Science Statement - A Future Made in Australia, 2024.

> [FT27 TODO] confirm these policies are still current/announced at FT27 lodgement; add any newer ones.

E2. Research Activity Type

Item	Response
Applied research (%)	10
Pure basic research (%)	50
Strategic basic research (%)	40

E3. Field of Research

Code	Name	Percentage
401804	Nanoelectronics	30
510805	Quantum technologies	30
510403	Condensed matter modelling and density functional theory	40

E4. Socio-Economic Objective

Code	Name	Percentage
240403	Integrated circuits and devices	20
280110	Expanding knowledge in engineering	20
280120	Expanding knowledge in the physical sciences	60

E5. Interdisciplinary Research

FT26 reference: up to 375 characters; approximately 50 words.

Disorder-oriented materials design requires strong integration of knowledge from materials science and condensed matter physics, with progress driven by advanced computational methods. Achieving meaningful outcomes in model construction, materials screening, and device modelling further depends on inputs from algorithm development and artificial intelligence.

Yes - Investigatory Team, Methodology, Design

E6. International Collaboration

Yes

E7. Countries Involved in International Collaboration

- United States of America
- New Zealand
- Japan

E8. Research Student Places

Item	Response
PhD (FTE)	2
Masters (FTE)	0
Honours (FTE)	3

Part F - Project Eligibility

F1. Medical Research

No

F2. Medical Research Statement

FT26 reference: up to 750 characters; approximately 100 words.

Not completed / blank in the working data.

Certification status

Not certified. The certification pages of the historical submitted application are not evidence of approval of this FT27 draft. Certification and any declarations must be completed through the applicable institutional and RMS process.

Review Notes - outstanding FT27 updates

meta.status

DRAFT baseline carried from FT26. Part C (Project Description) and C2 (Letter of Support) are flagged for revision pending the applicant's instructions on the new perspective for FT27. Part D budget years and salary/stipend rates need re-indexing to a 2027–2030 commencement (currently still shows the FT26 2026–2029 figures verbatim).

form_fields.B9_mentoring_leadership.note

[FT27 TODO] Confirm supervision, publication and presentation counts; condensed from FT26 evidence.

form_fields.B10_research_output_context.note

[FT27 TODO] update publication/citation/h-index counts to current figures before submission.

form_fields.B12_current_arc_projects.note

[FT27 TODO] Refresh from the participant's current RMS record.

form_fields.B14_eligibility_extension.note

Historical FT26 answer; confirm against FT27 eligibility dates and current certification.

form_fields.B17_professional_equivalent_to_phd.note

[FT27 TODO] The source PDF page 11 records Yes even though B13 lists a PhD. Confirm this response with the Research Office; retained faithfully here.

form_fields.E1_government_priority_areas.note

[FT27 TODO] confirm these policies are still current/announced at FT27 lodgement; add any newer ones.

reference.B11_note

[FT27 TODO] review for any papers published since Nov 2025 that should displace a weaker entry; recompute h-index/citations in B10 to match.

reference.D1_budget.note

[FT27 TODO] These are the verbatim FT26 figures (commencing 2026, so effectively 2026-2029). For FT27 (commencing 2027), re-index: (1) shift the four years to 2027-2030, (2) update Dr Yin's Level B salary point and on-costs to the rate current at FT27 lodgement, (3) update the ARC HDR stipend rate for the relevant year, (4) re-check conference years/venues in the travel plan (D2) still make sense for a 2027 start, (5) recompute all year and grand totals once rates are updated.

parts[0].status

carried from FT26 — figures/amounts inside may need refreshing (see notes)

parts[0].sections[0].blocks[5].note

[FT27 TODO] Confirm the cumulative NCI/Pawsey allocations and valuations; these are FT26 figures.

parts[1].status

FT26 research baseline; figures restored; FT27 research direction awaits applicant input

parts[2].status

carried from FT26 — needs re-dating and reissue by Monash Research Office for FT27

parts[2].sections[0].blocks[0].note

[FT27 TODO] replace with new letter date once reissued for the FT27 round.

parts[2].sections[0].blocks[6].note

[FT27 TODO] refresh ERA/QS ranking citations if newer editions are out by FT27 lodgement.

parts[3].status

carried from FT26 — years/rates/conference plan need re-indexing to 2027-2030 (see D1 note) parts[3].sections[0].blocks[1].note

[FT27 TODO] confirm salary point/on-cost rate current at FT27 lodgement.

parts[3].sections[0].blocks[3].note

[FT27 TODO] confirm ARC HDR stipend rate for the FT27 round.

parts[3].sections[1].blocks[15].note

[FT27 TODO] recheck conference years/venues (AIP Congress, APS Global Physics Summit, MRS Spring, Gordon Godfrey Workshop) are still appropriately scheduled for a 2027-2030 fellowship.

parts[3].sections[2].blocks[3].note

[FT27 TODO] reprice VASP licence and workstation hardware at FT27-lodgement prices.

parts[4].status

carried from FT26 — dollar figures need re-indexing alongside D1/D2

Current round information: ARC notice dated 18 August 2026 schedules FT27 applications for 23 September to 6 November 2026. Verify the released round documentation.

Source: ARC scheme update - FT27