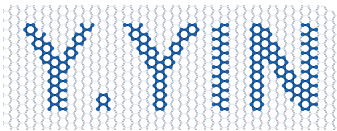


Response to Selection Criteria



Yuefeng Yin

AEA Ignite Project Lead / Research Fellow, Dept. of Materials Science and Engineering,
Monash University
yuefeng.yin@monash.edu · github.com/yyfforce

SUMMARY

I am a computational materials scientist with a PhD from Monash University and nine years of postdoctoral experience, including seven years with the ARC Centre of Excellence in Future Low-Energy Electronic Technologies. My research is built around a clear goal: use computation to identify promising materials, understand the physics behind their properties, and work with experimentalists to test whether those predictions hold in real materials and devices. This work directly aligns with the Digital-led Discovery and Design of New Materials Cluster.

Over this period, I have published 43 refereed articles, including 15 in the past three years and six in journals with impact factors above 10. I have worked with academic and industry partners to secure more than A\$3.4 million in research funding since 2024, including an AEA Ignite project that I lead and an ARC Linkage Project in which I am a Key Participant. I am also lead inventor on a US patent application.

Alongside my research, I have designed and delivered a university course in computational materials science, trained Master's and PhD students in density functional theory, and mentored nine PhD candidates. At UNSW, I would bring this combination of research, teaching, collaboration and translation to help build a shared Faculty-wide capability for digital materials discovery.

NOMINATED STRATEGIC RESEARCH CLUSTER
Cluster 1 — Digital-led Discovery and Design of New Materials

NOMINATED HOST SCHOOL
School of Materials Science & Engineering

LEVEL
Lecturer (Level B)
also open to Senior Lecturer (Level C)

My disciplinary home is materials science and engineering — thin-film design, structure–property relationships, and the computational methods that connect them — which is why I nominate the **School of Materials Science & Engineering** as my host School. My research practice, however, is interdisciplinary by construction: the design rules I develop are only useful once they are tested by experimental physicists, turned into synthesis targets by chemists, and made statistically robust by applied mathematicians. **Cluster 1** is the natural home for that work, and the reason I am applying to UNSW rather than continuing along a single-School trajectory elsewhere.

ALIGNMENT WITH THE ADVERTISED RESEARCH AREAS OF CLUSTER 1 — DIGITAL-LED DISCOVERY AND DESIGN OF NEW MATERIALS

CLUSTER RESEARCH AREA (AS ADVERTISED)	FIT	EVIDENCE FROM MY RECORD
Computational and multiscale materials modelling		Extensive experience in developing DFT, tight-binding, Wannier and transport models for materials and devices.
Functional and structural materials		Designed magnetic thin films, topological materials and two-dimensional systems for low-energy electronics.
Chemical and physical approaches to materials design		Developed composition, disorder and interface design rules validated through experiment.
High-throughput experimentation and screening		Led national HPC allocations for large-scale screening of structures, compositions and interfaces.
AI and machine learning for materials discovery		Developing AI agents that connect simulation, high-throughput data and experimental feedback.

core expertise

strong, demonstrated

emerging / building

5 of 9 advertised areas shown

SKILLS AND EXPERIENCE

KNOWLEDGE & SKILLS PROFILE

COMPUTATIONAL METHODS	THIN-FILM & FUNCTIONAL MATERIALS	QUANTUM MATERIALS	TEACHING & SCHOLARLY PRACTICE
- Density functional theory (DFT) - Tight-binding & Wannier modelling - Quantum transport & device modelling - Large-scale HPC (NCI & Pawsey; >3M SU as Lead CI)	- Heusler alloy thin films (Co_2MnX, X = Ga, Ge) - Amorphous & disordered magnetic films - Bismuth thin-film allotropes	- Topological pyrite-type materials - Magnetic topological insulators - Phonon–topology interactions	- Curriculum design & tertiary teaching - HDR supervision (9 PhD candidates) - Grant writing & manuscript preparation - Peer review & research translation

1 A PhD or equivalent qualification in a relevant discipline.

RESPONSE

I hold a **PhD in Materials Science and Engineering** from Monash University, awarded for a thesis on tailoring the electronic structure of graphene via molecular adsorption. My undergraduate degree is a B.Eng. in the same discipline, completed through the Monash–Central South University “2+2” program.

My qualification is directly relevant to the nominated Cluster and host School. My academic career has combined first-principles theory, structure–property reasoning and large-scale computation for atomically thin materials, closely aligning with the core strengths of Cluster 1. This trajectory has established me as an emerging computational materials scientist pursuing independent research with high-impact publications and competitive grant success. Looking forward, I aim to integrate physics-based modelling with data-driven and AI-enabled methods to accelerate materials discovery. I see computational materials science as a defining discipline of the AI era, capable of transforming how materials are discovered and engineered, and driving technological advances that will transform human life.

CAREER AT A GLANCE



2 Demonstrated research excellence in an area aligned with one of the Faculty's Strategic Research Clusters.

RESPONSE

My research demonstrates excellence in the Faculty's **Digital-led Discovery and Design of New Materials** cluster, particularly in AI-enabled materials discovery, high-throughput screening, and computational and multiscale modelling. I combine first-principles calculations, tight-binding and quantum-transport methods to identify functional materials, optimise their structures and interfaces, and predict their performance under realistic operating conditions.

I lead a systematic program to discover two-dimensional materials for low-energy electronics. My high-throughput simulations generate the validated datasets needed for machine-learning and surrogate models, providing a foundation for an AI-enabled materials-design workflow. This program has produced a US patent application, with another patent and publication in preparation, and attracted approximately **A\$3.4 million** in government and industry support, including a **A\$650,000 AEA Ignite award as Lead CI**. I coordinate a 10-person experimental and theory team and have built strong relationships across Australian and international quantum-materials communities.

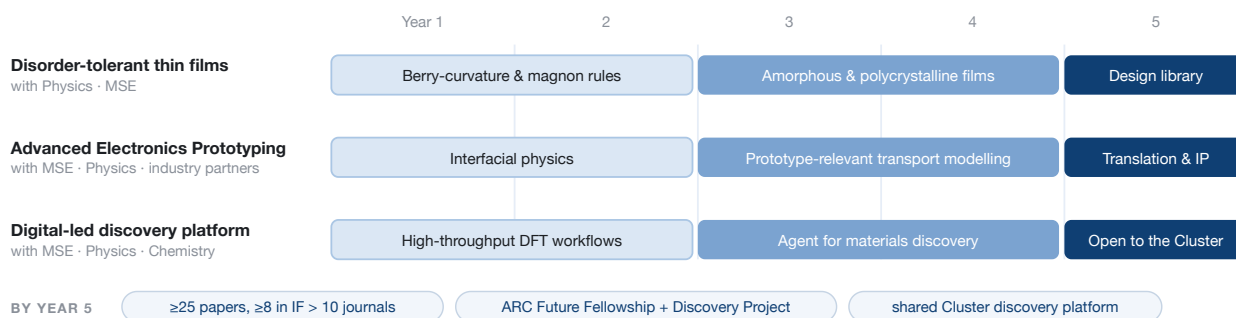
My multiscale modelling connects atomic structure with electronic, magnetic, optical and transport behaviour. Working closely with experimental physicists, chemists and materials scientists, I have shown that large Berry curvature survives complete structural disorder in amorphous Co_2MnGa , engineered spin-wave propagation through compositional control, and developed a sustained research program in two-dimensional bismuth allotropes, progressing from foundational theory to stabilising device-relevant topological edge states. Over the past three years, I have published **15 papers**, including first, co-first and corresponding-author work in Nature Communications,

Matter and Materials Today Physics, with key contributions to Advanced Materials and Nano Letters. My research has attracted **more than 1,200 citations**, approximately doubling its career impact over this period.

I have independently secured national Nectar cloud capacity and **more than three million NCI and Pawsey service units** as Lead CI. These resources sustain the development of high-throughput, data-driven modelling and the transition towards AI-assisted materials discovery. Together, my record demonstrates excellence through methodological innovation, high-impact discoveries, experimental collaboration, research leadership, competitive funding and translation into device-relevant intellectual property.

Below is my vision for the research program I would bring to the Cluster, how I would approach and benefit from interdisciplinary collaboration, and what I would deliver over the next five years:

THE RESEARCH PROGRAM I WOULD BUILD IN THE CLUSTER – THREE STREAMS, ONE SHARED COMPUTATIONAL PLATFORM



3 *Demonstrated ability and enthusiasm to contribute to interdisciplinary research and to actively participate in the development of a Faculty Strategic Research Cluster.*

RESPONSE

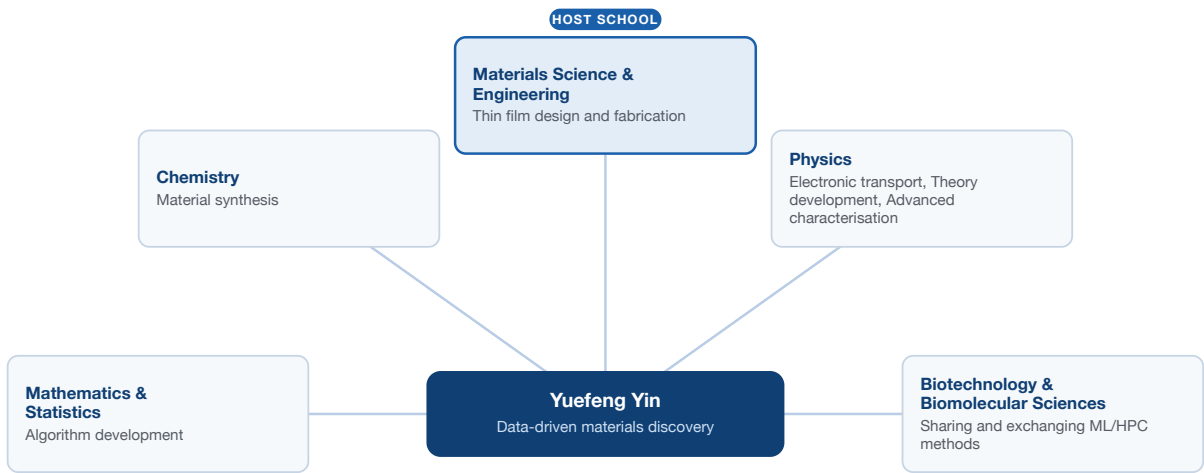
Interdisciplinary research is already how my work operates. I maintain close and productive connections across materials science, physics, chemistry, engineering and industry. My research is built around closing the loop between computational prediction, experimental validation and technology translation, with each discipline contributing knowledge that cannot be supplied by another.

In recent years, I have worked closely with researchers across Physics and Materials Science and Engineering to prototype advanced electronic technologies. Together, we investigate how semiconductor fabrication can benefit from our proposed materials and device architectures. This requires us to connect atomic-scale modelling with materials synthesis, interface engineering, device fabrication and performance testing. **Interdisciplinary knowledge and collaboration are indispensable to developing a robust understanding of whether a theoretical concept can operate in a manufacturable device.**

This experience has given me a clear view of what makes a research cluster effective. Shared infrastructure creates sustained collaboration. I would help develop a common high-throughput screening and surrogate-modelling platform that chemists, physicists, materials scientists and biomolecular researchers could apply to their own problems. My goal would be to contribute a capability that Cluster members use regularly to generate data, test ideas and initiate collaborative projects.

I would actively support the Cluster by convening regular computational modelling workshops, co-supervising HDR students across School boundaries, sharing computational infrastructure and expertise, and developing joint grant applications from their earliest stages. I would contribute expertise in materials physics, high-throughput computation and data-driven modelling, while benefiting from the Cluster's strengths in AI, statistics, chemistry, fabrication and experimental validation. This exchange would strengthen the Cluster's capacity to deliver ambitious, externally funded and experimentally validated materials discoveries.

HOW I WOULD WORK ACROSS THE CLUSTER'S SCHOOLS – WHAT I BRING, AND WHAT I NEED FROM EACH



4 Evidence of high-quality research outputs and the potential to develop an internationally recognised research profile.

RESPONSE

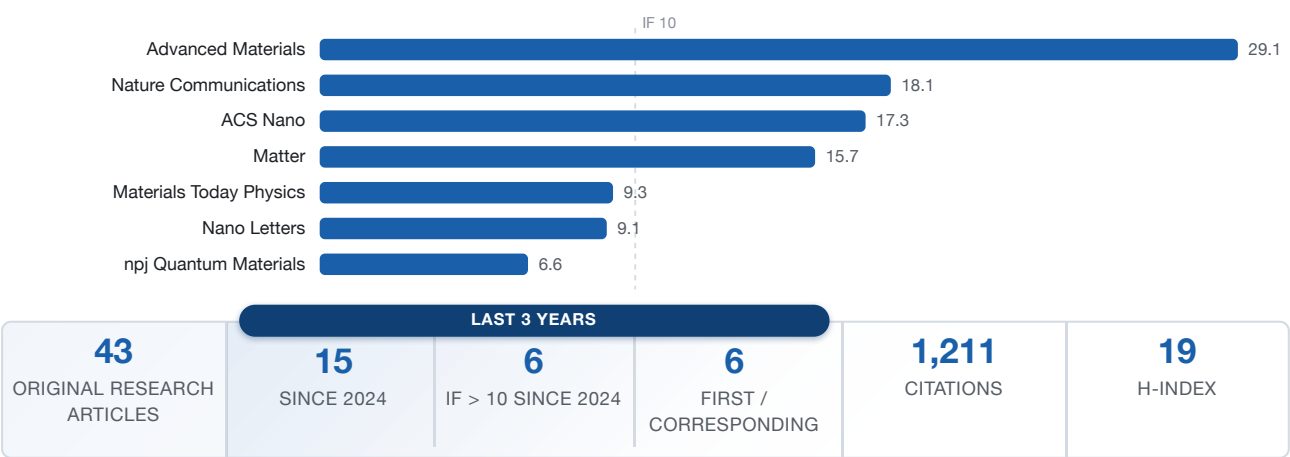
Research impact and momentum. My publication record comprises **43 refereed original research articles**, attracting **more than 1,200 citations with an h-index of 19**, as reported by my Google Scholar profile. I have published **15 papers in the last three years**, including **six in journals with impact factors above 10**. My citation count has more than doubled over the same period, demonstrating the growing visibility and influence of my research.

Leading high-impact research. I hold first, co-first or corresponding authorship on papers in **Matter, Nature Communications, npj Quantum Materials and Materials Today Physics**. In these studies, I shaped the research questions, developed the theoretical frameworks, directed the computational methodologies and interpreted the results. My work spans high-throughput materials discovery, topological and magnetic materials, electronic and spintronic transport, and device-relevant materials design.

Peer recognition and outputs beyond publications. I have presented at major international forums, including the American Physical Society March Meeting and the International Conference on Two-Dimensional Materials. I also review for Nature Communications and Communications Physics, demonstrating recognition of my expertise by leading journals. My broader research outputs include **a US patent application as lead inventor**, openly available research code and course materials, and public contributions to scientific knowledge.

A clear trajectory towards international recognition. I have established a strong national profile and a growing international research network across China, the United States, Japan and New Zealand, supported by sustained collaborations, research exchanges and joint projects. I will build on this network to establish a distinctive international program in digital-led materials discovery, attract competitive fellowships and research funding, train HDR researchers, and lead collaborations that translate computational predictions into experimentally validated materials and technologies.

SELECTED VENUES OF MY REFEREED PUBLICATIONS – JOURNAL IMPACT FACTOR



5

Demonstrated ability, or clear potential, to attract competitive research funding.

RESPONSE

Proven funding success. Since 2024, I have contributed to securing **more than A\$3.4 million** in competitive government and industry research funding, in roles ranging from Key Participant and Co-CI to Lead CI. Most notably, I secured **A\$650,000** through Australia's Economic Accelerator Ignite program **as Lead CI** for From Lab to Fab: Advancing a New Low-Energy Transistor Towards Large-scale Manufacturing. I developed and led the application, demonstrating my ability to articulate both the scientific significance and commercial potential of my research to reviewers beyond my discipline.

Government and industry partnerships. I am a Key Participant in a **A\$1.7 million** ARC Linkage Project developing a low-energy topological transistor, in partnership with TQ Transistors. I am also a Co-CI on **A\$1.04 million** in industry funding for materials design and prototyping of negative-capacitance field-effect transistors. These projects demonstrate my ability to build interdisciplinary partnerships, align fundamental research with industry priorities, and develop competitive proposals with clear pathways to translation.

Competitive computational resources. As Lead CI, I have independently secured major national computing allocations through the **NCI Adapter Scheme**, the **NCI-Monash Computational Scheme** and the **Pawsey Fast Track Scheme**. These separately peer-reviewed awards provide the computational capacity required for high-throughput materials screening, multiscale modelling and data-driven discovery.

A strong funding pipeline. My next step is to build on this record as lead investigator of nationally competitive research programs. A continuing appointment would position me to lead ARC Discovery Project applications and pursue an ARC Future Fellowship. My first Discovery Project concept, focused on disorder-tolerant functional thin films, is already developed in outline. This combination of demonstrated funding success, industry engagement and a clearly defined research pipeline provides a strong foundation for sustained competitive funding.

COMPETITIVE RESEARCH FUNDING — SECURED SINCE 2024, AND THE PIPELINE I WOULD RUN AT UNSW

SECURED SINCE 2024 — A\$3.39M ACROSS THREE SCHEMES

ARC Linkage Project — LP250200919	Key Participant	A\$1.70M
Industry R&D — TQ Transistors	Co-CI	A\$1.04M
AEA Ignite Round 2 — IG250200225	Lead CI	A\$0.65M

Plus >3M service units of national HPC won as Lead CI (NCI Adapter Scheme; Pawsey Fast Track).

FIVE-YEAR COMPETITIVE FUNDING AND PARTNERSHIP ROADMAP AT UNSW

Year 1

Establish independent leadership

- NCMAS national HPC allocation as Lead CI
- ARC Discovery Projects 2028 application
- ARC Explore proposal for high-risk, high-reward materials discovery
- UNSW and Faculty seed funding for interdisciplinary pilot projects

Years 2–4

Scale national and international partnerships

- ARC Lead and Mentor application
- ARC Collaborate and Breakthrough proposals
- Participation in industry-led CRC-P and translational research bids
- Bilateral and multinational projects across China, the United States, Japan and New Zealand

Year 5

Lead a major research consortium

- Participate in an ARC Prioritise or equivalent centre-scale proposal
- Establish an international consortium in AI-enabled materials discovery
- Secure sustained government, industry and international co-investment

6

Evidence of effective teaching and a commitment to delivering an outstanding student experience.

RESPONSE

Proven course design and delivery. I have six years of undergraduate and postgraduate teaching experience. As Lecturer in Computational Materials Science at Central South University, delivered through the Monash and CSU 2+2 program, I designed the course from the ground up. I developed the curriculum, lectures, tutorials and assessments, covering condensed-matter fundamentals, density functional theory, high-performance computing and applied modelling. The complete course materials are openly available on GitHub.

Research-led postgraduate training. I regularly deliver DFT workshops and tutorials for Master's and PhD students at Monash. My focus is not simply on running software, but on helping students select, justify and validate the computational method appropriate to their research question.

A clear teaching philosophy. I teach physical principles and reasoning before software implementation, giving students knowledge that remains useful as computational tools evolve. I make abstract concepts accessible through interactive visualisation, worked examples and authentic research problems. This approach develops both technical competence and the confidence to apply knowledge independently.

Contribution to UNSW. I would contribute immediately to computational and materials-science teaching while developing new learning opportunities in **AI-assisted materials design**. This emerging area offers a distinctive opportunity to connect fundamental materials science with computation, data science and contemporary research practice.

7

Demonstrated ability to collaborate across disciplines and build productive research partnerships.

RESPONSE

Collaboration is central to how I deliver research. I build partnerships across disciplines, institutions and sectors, then convert them into high-quality publications, competitive funding, shared capability and research translation.

Across disciplines. My collaborators include physicists, chemists, materials scientists, engineers and industry specialists. In my recent advanced-electronics work, I coordinate a 10-person team connecting first-principles modelling with materials synthesis, device fabrication, performance testing and commercialisation. My role is to establish shared research questions, translate concepts across disciplines and ensure that computational predictions address practical fabrication and device requirements.

Across institutions and sectors. I have sustained a long-term partnership with Victoria University of Wellington through joint projects, publications and reciprocal visits. I also maintain active collaborations with researchers at RMIT and other Australian and international institutions. Beyond academia, I work closely with TQ Transistors on low-energy electronic technologies and am lead inventor on a US patent application. I also helped develop the Monash and Jiangxi Copper partnership from initial contact to a formal Memorandum of Understanding.

I sustain productive partnerships by agreeing on objectives and responsibilities at the outset, communicating regularly, and recognising each partner's contribution fairly. This approach has enabled my collaborations to continue across multiple projects and several years, demonstrating my ability to build relationships that deliver lasting scientific, translational and institutional value.

8

Experience in supervising, or the capacity to supervise, Higher Degree Research students.

RESPONSE

Established supervision experience. I have mentored or co-supervised **nine PhD candidates**, including five graduates and four current candidates. I have also supervised three Bachelor's and Master's research students and examined two PhD theses within my Department. This experience has prepared me to take full responsibility as a principal HDR supervisor.

Developing independent researchers. My goal is to develop students who can identify, test and defend their own research questions. I provide close guidance during the first project, often working through calculations alongside the student, then progressively transfer responsibility for methodological and research decisions. I also train students to challenge their own conclusions, because a computational result is not robust until its assumptions and limitations have been tested.

Strong student outcomes. Researchers I have mentored have progressed to first-author publications in Advanced Science, ACS Nano and Nano Letters. One former candidate now holds a joint postdoctoral appointment at the **University of Cambridge and King's College London**. These outcomes demonstrate my ability to support both high-quality research and long-term career development.

At UNSW, I would build a focused group of three to four HDR candidates within five years. I would actively pursue cross-School co-supervision within the Cluster, particularly with colleagues in statistics, AI, chemistry and experimental materials science. Joint supervision would give students genuinely interdisciplinary training while creating durable research connections across the Faculty.

HIGHER DEGREE RESEARCH SUPERVISION AND EXAMINATION TO DATE



5 – PhD graduated
co-supervised / mentored



4 – PhD in progress
currently mentoring



3 – Bachelor's / Master's
research projects supervised



2 – PhD theses examined
Departmental examiner

Mentees have first-authored papers in Advanced Science, ACS Nano and Nano Letters.

One graduate now holds a joint postdoctoral appointment at the University of Cambridge and King's College London.

9

Excellent interpersonal, communication and organisational skills.

RESPONSE —

My research depends on coordinating people with different expertise, priorities and measures of success. I communicate complex ideas clearly, organise multidisciplinary projects effectively, and build productive relationships through preparation, listening and reliable follow-through.

- **Communication across audiences.** I communicate research clearly to physicists, engineers, intellectual-property professionals, students and the public, adapting the technical depth while maintaining accuracy. I have also contributed to quantum-science outreach through Melbourne Knowledge Week and FLEET.
- **Organisation under constraints.** I lead a A\$650,000 advanced-electronics translation project involving two Schools, an industry partner, a substantial budget and formal scientific and commercial milestones. I also manage more than **three million** national computing service units, requiring careful planning, monitoring and reallocation.
- **Preparation that enables partnerships.** For Monash's engagement with Jiangxi Copper, I identified relevant expertise across three departments, approached academics individually, and briefed both sides before formal discussions. This preparation helped focus the engagement on concrete research opportunities and contributed to a formal Memorandum of Understanding.
- **Constructive decision-making.** In multidisciplinary project meetings, I seek to understand each participant's position before presenting my assessment. This approach builds trust, resolves differences efficiently and supports decisions that partners can implement collectively.

10

Demonstrated commitment to equity, diversity and inclusion, and to fostering a respectful and collaborative academic environment.

RESPONSE —

I am an international academic who came to Australia as an undergraduate through a joint degree program. Much of my career has involved working across academic cultures with different expectations around hierarchy, disagreement and recognition. This experience shapes how I create an inclusive and respectful research environment.

Making expectations explicit. Practices such as approaching collaborators, questioning senior colleagues and determining authorship are often communicated informally. This can disadvantage students unfamiliar with the academic system. I explain these expectations clearly and support students in developing the confidence to participate fully. My **nine PhD mentees** have represented diverse nationalities, genders and academic backgrounds.

Lowering barriers to computational research. Computational materials science can appear inaccessible to students without extensive programming experience or computing resources. I make course materials and research code **openly available** and teach students to begin with physical reasoning before developing software skills.

Ensuring credit and visibility. I recognise contributions transparently and support junior researchers in taking ownership of their work. My mentees have published first author papers in Advanced Science, ACS Nano and Nano Letters, reflecting both their intellectual contribution and my commitment to ensuring appropriate recognition.

Fostering respectful collaboration. I establish clear expectations for communication, responsibilities and authorship at the beginning of each project. I encourage students and colleagues to question ideas regardless of seniority and address disagreements directly and respectfully. This allows different perspectives to strengthen the research.

I am committed to upholding the UNSW Code of Conduct and Values and to fostering an environment in which every colleague and student is treated with fairness, dignity and respect.

11

Knowledge of health and safety responsibilities and commitment to attending relevant health and safety training.

RESPONSE —

I understand that health and safety is a shared responsibility applying to every staff member, not only those working directly in laboratories. It includes physical safety, psychological wellbeing and the obligation to ensure that my actions do not place others at risk.

- **Current practice.** I have completed the mandatory health and safety training required for my current role and comply with University policies and procedures. Although my research is primarily computational, I work alongside experimental laboratories and follow all local safety and access requirements.
- **Safe work environments.** I respond promptly to workplace safety requirements, seek clarification when needed and take appropriate action. This includes maintaining a safe workspace, following reasonable instructions and reporting potential hazards or concerns through the correct channels.

- **Supervisory responsibility.** As an HDR mentor, I recognise workload, deadline pressure and the isolation associated with computational research as genuine wellbeing risks. I maintain regular contact with students, set realistic expectations and address concerns before they escalate.
- **Commitment at UNSW.** I would complete all required UNSW inductions and mandatory training upon commencement, maintain current refresher training and undertake any additional instruction required by the host School or laboratories with which I collaborate.