Response to

Selection Criteria

for Lecturer/Senior Lecturer – Theoretical Quantum Physics, Monash University

Yuefeng Yin

SC: Selection Criteria

SC: *A PhD degree in Materials Science and Engineering, Physics, Chemistry or a relevant discipline.*

Response: I received my **PhD degree in Materials Science and Engineering** from Monash University.

As a PhD graduate specializing in the theoretical modeling of functional materials, my research background is closely aligned with the field of computational materials science. Following my PhD, I joined the ARC Centre of Excellence in Future Low-Energy Electronic Technologies (FLEET) as a postdoctoral fellow. In this role, I have continued to advance my computational modeling skills, work and collaborate in a highly interdisciplinary environment, and actively participate in a range of research and teaching activities.

SC: *Demonstrated experience in relevant computational techniques and associated tools (examples include, but are not limited to machine learning, density-functional-theory, materials informatics, finite-element modelling, phase-field modelling), and demonstrated broad-range of applications in materials research.*

Response: I have extensive experience in the field of computational materials science, with a rich background in various modeling areas including, but not limited to, density functional theory (DFT), molecular dynamics, tight-binding modeling, high-throughput data extraction, and machine learning.

As reflected in my CV, my main expertise lies in the DFT approach, where I have applied DFT modeling to address problems in metals and alloys, semiconducting materials, and low-dimensional materials, targeting a broad range of applications in electronics, spintronics, energetics, and catalysis.

In recent years, I have shifted my focus toward integrating the latest developments in data science and machine learning with DFT and tight-binding methods. I believe that in the next decade, the trend of “AI for Science” will fundamentally transform the way we conduct materials research.

My experience and achievements can be briefly summarized in the following highlights.

- The majority of my calculations occurred during my tenure in the ARC Center of Excellence in Future Low-Energy Electronic Technologies (FLEET), with a consistent focus on applying DFT modeling and tight binding models to investigate the electronic and spintronic structure of low-dimensional quantum materials. (See examples: prediction of novel spintronic materials in pyrite compounds and electronic properties of amorphous topological materials.)
- My expertise in low-dimensional materials enables me to investigate the sensing and catalytic performance of atomically thin films thorough independent research and collaboration with experimental groups.(See examples: biosensing using graphene and planar molybdenum oxide for enhanced alkaline hydrogen evolution.)
- In recent years, through collaborations with industrial partners, I have further applied my computational materials science expertise to the field of advanced manufacturing, with a focus on potential applications in aerospace and transistors.

SC: *A strong track record in independent and cross-disciplinary collaborative research with outcomes of high quality and high impact as demonstrated by high-quality publications, particularly in computational techniques applied to materials research.*

Response: As of May 4, 2025, my research career has been marked by significant achievements in the field of 2D materials and topological materials. I have published 36 papers in peer-reviewed journals, with an additional 3 papers currently under review and 2 papers in preparation. My publications have received 859 citations, resulting in an h-index of 16. My publications showed a consistent history of delivering original high-quality research in interdisciplinary studies, as well as demonstrating my ability to work within a research team of diverse backgrounds. You can verify my history of publications and citations in Google Scholar through the following link: Google Scholar Profile.

Here is the summary of highlights:

- **High-quality original computational materials modeling**: My journey in the field of computational materials modeling started during my PhD, with a focus on the electronic structure of graphene. My PhD work was published in reputable journals such as the Journal of Physical Chemistry C and the Journal of Physics Letters. After joining the ARC Centre of Excellence in Future Low-Energy Electronic Technologies (FLEET), I continued to produce innovative research on topological insulators and spintronics, which was published in prestigious journals such as ACS Nano, npj Quantum Materials, and Matter.
- **Development of novel computational modeling techniques to break the scale limit of DFT calculations**: In addition to using existing DFT implementations to simulate materials properties, I have developed new algorithms and codes to improve computational efficiency in electronic structure calculations and to overcome limitations of current modeling approaches. These developments have opened new horizons for computational materials science. Some of these algorithms have been featured in my recent publications in Materials Today Physics and Nano Letters.
- **Maintaining a focused research topic based on interdisciplinary knowledge**: My research career has revolved around investigating the electronic and spintronic structures of low-dimensional materials using computational methods. While rooted in materials science, this research topic necessitates interdisciplinary knowledge for achieving outstanding publication records. Throughout my career, I have developed expertise in physics, chemistry, computer science, and mathematics, and applied these interdisciplinary skills to contribute to publications in physics- and chemistry-focused journals. Furthermore, this diverse knowledge base has proven pivotal in collaborations with researchers from different backgrounds.

SC: *A demonstrated track record of securing research support from competitive grant schemes and industry.*

Response: I have a strong record of securing research support from competitive grant schemes and industry, as demonstrated by:

- During my tenure at FLEET, I was awarded a seed fund of 10,000 AUD by the Centre to conduct collaborative research with the MacDiarmid Institute in New Zealand.
- Since 2023, my project titled “Developing packages for simulating electronic and spintronic properties of amorphous materials” has received continuous computational support from the National Computational Infrastructure (NCI) Australia. To date, the accumulated computational hours granted exceed 3 MSUs (with an estimated cash value of 120,000 AUD under current NCI guidelines).
- In 2024, I arranged and led negotiations with a Fortune 500 company to establish a strategic partnership with Monash University through the signing of a memorandum of understanding. In 2025, I secured 1,000,000 AUD in research funding to carry out two industry-focused collaborative R&D projects.

- Also in 2024, I participated in securing 600,000 AUD in funding for two years from a start-up industrial partner to establish a modeling program focused on advanced electronics.

SC: *A demonstrated ability to work positively and cooperatively in a teaching and research-intensive environment, including across disciplines.*

Response: I have a consistent track record of working in a teaching and research-intensive environment during my time at Monash University. I believe in the importance of maintaining a positive and cooperative attitude when interacting with colleagues, which helps me remain confident and effective under the pressure of managing multiple ongoing research and teaching projects.

The nature of my expertise—computational modeling—has required me to work closely with fellow researchers and staff across disciplines. In my past experience, I have successfully delivered research and teaching assignments involving the Civil, Chemical, and Mechanical Engineering departments within the Faculty of Engineering, as well as the School of Physics in the Faculty of Science.

I can provide some examples of how this work manner helped me to achieve success:

- During my tenure at the ARC Centre of Excellence in Future Low-Energy Electronic Technologies (FLEET), I worked closely with physicists, materials scientists, and chemical scientists on interdisciplinary projects. In one study, we investigated the electronic properties of magnetic topological materials using DFT calculations to provide theoretical explanations for experimental data. Our success relied on open communication, mutual respect for disciplinary expertise, and a shared vision of research outcomes. Collaborations like these not only led to high-impact publications but also enhanced my ability to adapt and contribute across disciplines.
- While coordinating courses for the Monash–Central South University "2+2" exchange program, I worked with colleagues across a range of materials disciplines (e.g., metals and alloys, polymers). Together we designed and delivered content that integrated condensed matter physics, materials engineering, and computational modeling, seamlessly blending each colleague's expertise. This experience enhances my ability to collaborate within a teaching team that spans a broad spectrum of expertise.

SC: *A demonstrated ability to undertake quality teaching of both introductory and specialist courses at undergraduate and postgraduate level.*

Response: I have the ability to teach introductory specialist courses at every degree level. At the undergraduate level, I have extensive experience delivering computational materials science courses at Monash University. These classes begin with core concepts in condensed matter physics and computational modeling formalisms and finish with projects that apply these techniques to practical materials science problems. At the postgraduate level, I have experience running DFT training workshops and tutorials for master's and PhD students, helping them understand modeling principles and choose suitable computational approaches for their research.

SC: *A demonstrated ability to develop quality curriculum in disciplines such as computational and machine-learning in material science, physical properties of materials.*

Response: I have experience in developing curricula related to computational materials science and the electronic properties of materials, incorporating the latest developments in the field, such as data science and machine learning.

As an example, I can provide the outline of a 12-week "Computational Materials Science" course that I designed.

Brief Course Information

Course Name	Computational Materials Science
Course Type	Elective course for 3rd or 4th undergraduate year
Course Requirement	Numerical Analysis for Engineering; Engineering Mathematics
Reference Materials	1. David Sholl, Janice A. Steckel. *Density Functional Theory: A Practical Introduction*. Wiley, 2009. 2. Richard M. Martin, *Electronic Structure: Basic Theory and Practical Method*. Cambridge University Press, 2004.
Course Summary	This course introduces the application of computational modeling to address challenges in materials science and engineering. Density Functional Theory (DFT) serves as an example method for examining the physical and electronic characteristics of solids. The curriculum includes an overview of high-performance computing and the standard procedures for conducting atomic simulations. The conclusion of the course will feature an overview of recent advancements in computational materials science, including the integration of artificial intelligence to expedite materials design.
Course Assessments	Oral presentations / Mini project / Final exam

Course Schedule, Content and Assessment

Week	Lectures/Tutorials	Title	Content
1	2	Introduction to Computational Materials Science	1. What is computational materials science? 2. Advantages of modeling in materials science 3. Different approaches to materials modeling.
2	2	Demo: Monte Carlo Simulations	Using Monte Carlo simulation to demonstrate solving material properties.
3	4	Introduction to Atomic Simulations and DFT	1. Basics of atomic-scale simulations 2. What DFT can and cannot do 3. Examples of DFT capabilities
4	4	DFT in Action	1. Standard procedures for DFT (incl. atomic model building) 2. Linking computational results with experiments 3. From DFT theory to software practice

Week	Number of Lectures/Tutorials	Title	Content
5	2	High-Performance Computing (HPC)	1. What is HPC? 2. How to run DFT on supercomputers
6	4	Demo: DFT Calculations	Solving a real materials science problem using DFT (incl. HPC workflow)
7	2	Computational Materials Science for the Future	1. Advancements beyond DFT 2. Big data, AI and their roles in materials research
8	4	Demo: A Mix of Methods	Multi-scale and hybrid simulation techniques to solve materials problems (incl. machine learning).

- Assessment 1: Oral presentation in Week 6 — A mini review that analyzes how DFT modeling is used to solve specific problems in materials science.
- Assessment 2: Mini project from Week 9 to Week 12 — Practical application of DFT software and programming skills to address challenges in materials science.
- Final exam.

SC: *A demonstrated experience in course or program coordination and administration.*

Response: Despite being a research-focused staff member for years, I have gathered extensive experience in program coordination and administration:

- Played a significant role in coordinating courses targeted at "2+2" students enrolled in the Monash–Central South University exchange programs.
- Coordinated high-level international visitors coming to Monash University for official visits, including delegations from Central South University, Wuhan University of Technology, and Shanghai University.
- Coordinated collaborative research programs with established companies and start-up industrial partners.

SC: *The ability to apply new and innovative methods for teaching including the capacity to use current and new technologies for delivery in a flexible learning environment.*

Response: I am dedicated to transforming tertiary education into a more modern and digital format, aiming to equip students not only with knowledge but also with the necessary skills to adapt to the ever-evolving working environment, which has been significantly impacted by the emergence of artificial intelligence in recent years.

My experience of teaching computational modeling at Monash University is a perfect example demonstrating my approach of incorporating visualized models, interactive plots, and other digital mediums to showcase the impact of theoretical simulations in materials research. Through vivid digital notes, students gain a clear understanding of how abstract computational concepts can be applied to investigate material properties and

aid in material design. My teaching is well-received by students, who not only appreciate the capabilities of computational modeling by the end of the course but also acquire essential skills for their future careers.

SC: *Excellent interpersonal, oral, and written communication skills appropriate for interacting effectively with team members, collaborators and colleagues, including the ability to clearly write project and operational documents, produce online contents and contribute to meetings. This includes an ability to communicate well with people of diverse backgrounds and knowledges in research, computing, and management.*

Response: Years of working in an academic environment have sharpened my interpersonal, oral, and written communication skills. I have maintained excellent working relationships with fellow team members, academic staff, and professional personnel throughout my research career. I take pride in my professional and respectful attitude when interacting with supervisors and peer researchers. I am a good listener and always strive to communicate my concerns effectively with colleagues to ensure that the project progress always stays on the right track.

These capacities can be demonstrated by the following highlights in my career:

- Collaborate with FLEET operational staff to produce outreach materials promoting quantum science to the general public, including participation in Melbourne Knowledge Week. Some of these materials were shared via FLEET's social media channels including X and YouTube.
- Work with Monash staff and fellow researchers from diverse backgrounds to write articles promoting my research in both print and online media, such as Materials Australia magazine, the ARC Newsletter, and NCI Annual Reports.
- Coordinate with Monash staff across various departments to organize visits by high-level delegations from international institutions and companies.

SC: *Demonstrated experience of successful student supervision including but not limited to PhD, Honours, Masters, Vacation Scholars projects.*

Response: I have a long and successful record of supervising students of various degree levels and academic background, including:

- Served as co-supervisor of one PhD student (recently graduated from Monash University), and as part of the supervision team for five PhD students, resulting in two publications as corresponding author and five co-authored papers.
- Served as the main and co-supervisor for Research Master and Undergraduate students. Successfully transformed an undergraduate final year project into a well-cited publication with me as the corresponding author (see Li, Q., Smith, J.S., Yin, Y., Wang, C., Klymenko, M.V., Cole, J.H., Medhekar, N.V., Localized Wannier function based tight-binding models for two-dimensional allotropes of bismuth, New Journal of Physics, 2021, 23, 063042).
- Acted as mentor to several exchange students from Central South University, China, who joined Monash University to complete their final year projects.

SC: *An understanding of and commitment to UNSW's aims, objectives, and values in action, together with relevant policies and guidelines.*

Response: I understand the objectives, objectives and values of UNSW, and I am committed to upholding them in all aspects of my work. I will adhere to the relevant university policies and guidelines and ensure that my work conducted in UNSW is in line with the expectations and standards of this world-class institution.

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

Response: I am committed to fulfilling the health and safety responsibilities associated with this position, including attending relevant training sessions. I am fully aware of the potential health and safety risks related to desk work and am knowledgeable about ergonomic workspace design.