B8 — ROPE: Evidence of Research Impact and Contributions to the Field

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.