

Yuefeng Yin | Research Statement

Interfaces create properties that neither material possesses alone. They decide whether a quantum state survives integration, and whether a contact in a **low-energy transistor** — the hardware that sets the energy cost of computing, AI included — can both switch and conduct. I understand and design interfaces with first-principles and localised quantum models, alongside experiment and industry. At Sydney I would build **First Contact**: a program that turns interface physics into **a physical language that AI can learn from, generate with and be tested against**.

Interfaces, and why AI needs physics

Interfaces can reverse semiconductor polarity or improve carrier injection, and machine-learning models can now propose favourable interface configurations. But **a successful configuration does not establish which interactions caused its response**, whether they can be recreated elsewhere, or how much variation they tolerate — so AI-designed interfaces can be neither trusted nor reproduced. My program asks **which interactions are necessary, when they are sufficient, and where the description transfers**, and expresses the answers in a form that learning and generative methods can use and physics can test (right).

Track record

After a PhD (Monash, 2016) and seven years in the ARC Centre of Excellence FLEET, I have built an independent program on surfaces, interfaces and disorder across 46 refereed articles.

Original interface methods. I developed approaches that connect first-principles calculations with efficient localised models, and showed how surrounding layers and interface symmetry control the states of two-dimensional bismuth — weak substrate coupling and symmetric encapsulation each preserve its edge states (*New J. Phys.* 2021; *Mater. Today Phys.* 2023, 2025).

Interfaces in real devices. Our pick-and-place transfer of arbitrary-metal electrodes connects atomic interactions with van der Waals device fabrication (*ACS Nano* 2025, co-first). As Lead CI of the **A\$650K AEA Ignite** project and lead inventor on its US patent application, I am taking an engineered transistor channel towards manufacturing with TQ Transistors. With experimental partners I showed that giant Berry-curvature responses survive complete structural disorder (*Matter* 2025, co-first; *Nature Communications* 2026, co-first).

Preliminary foundation. My TQ Transistors programme adds interface design, **agent-assisted coding and high-throughput screening**. Its completed calculations (Figure 1) reveal the opportunity: assembly narrows the zero-field gap from 1.78 eV to about 0.4 eV, yet the complex stack retains a far stronger field response than the bare bilayer.

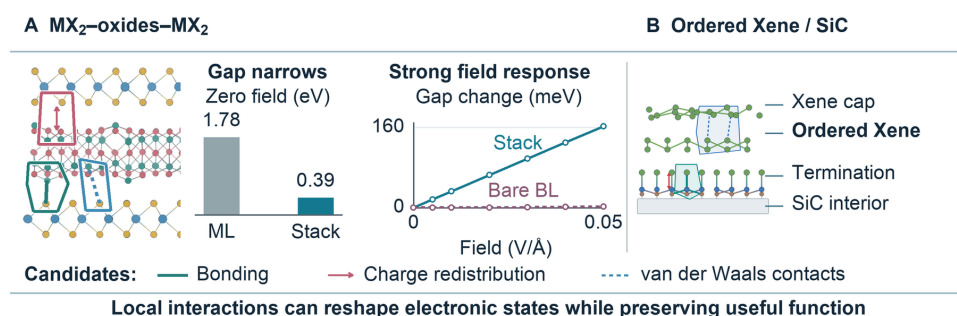


Figure 1. Local interactions reshape electronic states while preserving function. (A) MX₂-oxides-MX₂: reconstruction coexists with a strong field response; colours mark candidate interactions. (B) Ordered Xene / SiC: an ordered active layer under a lower-symmetry overlayer (illustrative).

46

refereed articles · h-index 20

A\$3.4M

research funding since 2024

Lead CI

AEA Ignite, A\$650K

>3M

national HPC units as Lead CI

9

PhD researchers co-supervised or mentored

AI IN FIRST CONTACT

UNDERSTAND AI

Does physics help learning?

Matched atomic-graph comparisons test whether Feature Zones improve compression and transfer — and when grouping discards information.

BUILD AI

Physics-conditioned generation

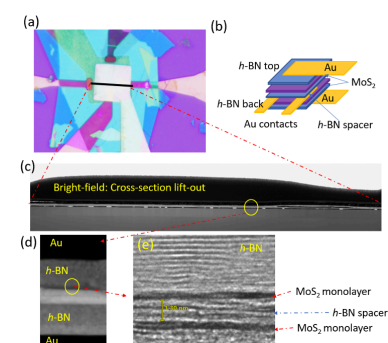
Zone requirements guide graph-based proposals, assembled in 3D under physical constraints and verified by DFT.

LEVERAGE AI

Agent-assisted discovery

Supervised AI agents build perturbation ensembles and reproducible analyses; OpenAI academic researchers cohort.

INTERFACES, ATOM BY ATOM



A van der Waals device lifted out by focused ion beam: STEM and TEM resolve every layer of the interface (AEA Ignite).

SELECTED LEAD-AUTHOR PAPERS

Pick-and-place transfer of arbitrary-metal electrodes — *ACS Nano* 2025 (co-first)

Giant Berry curvature in amorphous Co₂MnGa — *Matter* 2025 (co-first)

Edge-state control in 2D topological crystalline insulators — *Mater. Today Phys.* 2025 (corr.)

Phonon interactions in Mg₃Bi_{2-x}Sb_x — *Nature Communications* 2026 (co-first)

Research program: First Contact

I hypothesise that **a compact group of interacting atomic environments, with specified surroundings, can explain and reproduce an interface response** — a **Feature Zone**, which may link a bonded termination, a weak van der Waals contact and an active layer (Figure 2). Three Aims over four years test this, and each is also a test of AI.

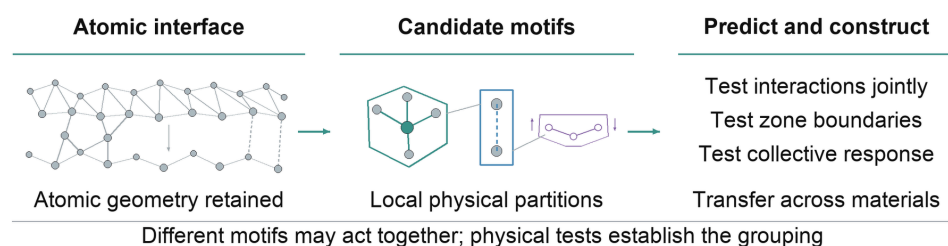


Figure 2. From atomic interface to Feature Zones. Candidate motifs proposed from the atomic geometry are tested jointly for their boundaries, collective response and transfer.

Aim 1 — Identify (*understand AI*). Perturbing motifs separately and jointly in a localised model, I will establish which interactions, surroundings and extent a response requires. **Matched atomic-graph comparisons** — Feature Zones against like-motif groups and unsegmented graphs, at equal inputs, training budgets and withheld configurations — will test **whether physical grouping improves learning**, and when it discards essential information.

Aim 2 — Construct (*build AI*). Mechanisms become requirements for termination, coordination and boundary fields. **Graph-based proposals** specify bonding and zone connections, assembled in 3D under chemical, geometric and periodic constraints and relaxed by first principles, and compared with conventional searches at matched cost. A candidate that keeps a motif but loses its function exposes a missing condition.

Aim 3 — Generalise (*leverage and test AI*). Responses and uncertainties will be **predicted for withheld material pairs before they are calculated**, then tested on larger, disordered interfaces with Green-function transport and published measurements — yielding tolerance maps of which variations preserve function.

AI in the workflow. Supervised AI agents will build perturbation ensembles, graphs and reproducible analyses under my validation, supported by my selection for **OpenAI's first ChatGPT for Academic Researchers cohort**. Code and data will be released through my open tool InterfaceHandler (InHand), so researchers and AI agents can reproduce every test.

Why Sydney, and outcomes

The program spans the Schools this Faculty brings together: **Computer Science** for graph learning and benchmarking; **Electrical and Computer Engineering** for contacts, transport and low-energy devices; **Chemical and Biomolecular Engineering** and **AMME** for interface assembly; and the **Sydney Nano Institute** and **Sydney Microscopy & Microanalysis** to test predictions against structure. Collaborators Simon Granville (VUW), David Cortie (Wollongong), Deep Jariwala (Penn State) and Bhaskaran Muralidharan (IIT Bombay) add disorder, interface and transport expertise. I have developed First Contact in full as an **ARC Future Fellowship** proposal, and would pursue it with ARC Discovery and Linkage funding while training two PhD researchers across materials physics and machine learning. Its outcome — tested principles for when interface function can be explained, recreated and predicted, with open code and data — will guide quantum-device integration and lower-energy electronics.

FOUR-YEAR PROGRAM

YEAR 1

Aim 1 · Identify Feature Zones

Mechanisms, boundaries, graph comparisons

M1 · mechanisms

YEARS 1.5–3

Aim 2 · Construct

Zone-conditioned generation, DFT relaxation

M2 · realisability

YEARS 2.5–4

Aim 3 · Generalise

Withheld pairs, scale, disorder, experiment

M3 · transfer limits

YEAR 4

Synthesis of principles

Two PhD theses; open code and data

M4 · synthesis

TWO DOCTORAL PROJECTS

PhD 1 · Bismuthene — environments that preserve or reconstruct its states; Ordered Xene / SiC as a bounded comparison

PhD 2 · Contacts — contacts combining carrier injection and electrical control, informed by the MX₂ stack

FUNDING SECURED SINCE 2024

ARC Linkage **A\$1.70M**

Key Participant

TQ Transistors **A\$1.04M**

Co-CI · industry

AEA Ignite **A\$0.65M**

Lead CI

Plus >3M NCI and Pawsey service units as Lead CI, and US\$12,000 OpenAI research support.

OUTPUTS

Linked papers on mechanisms, realisability and transfer — including cases that break the representation

Open code and reference data in **InHand**, reproducible by researchers and AI agents

Tolerance maps linking interface variation to preserved or lost function

PARTNERS

Sydney — Computer Science · Electrical & Computer Eng. · Chemical & Biomolecular Eng. · AMME · Sydney Nano · Sydney Microscopy & Microanalysis

International — S. Granville (VUW, NZ) · D. Cortie (Wollongong) · D. Jariwala (Penn State) · B. Muralidharan (IIT Bombay) · RIKEN links

Industry — TQ Transistors, with US partners