

First Contact

A Physical Language for Material Interfaces

Which interactions must an interface preserve
to retain its useful function?

Dr Yuefeng Yin

Department of Materials Science and Engineering, Monash University

Interfaces for quantum computing and advanced electronics

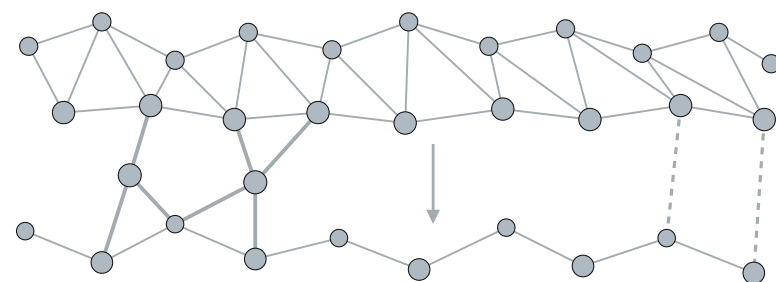
Quantum computing

Preserve useful quantum-material states as contacts and protective layers form around them.

Advanced electronics

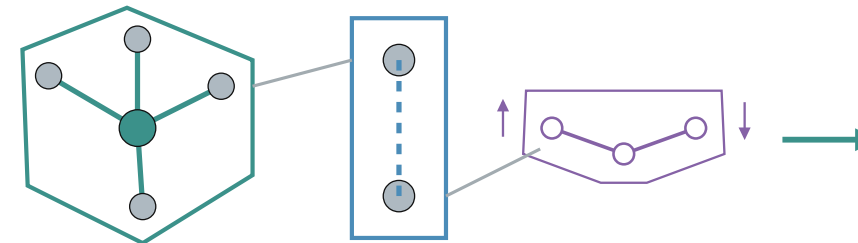
Use interface behaviour to improve electrical control and current flow in energy-efficient devices.

Atomic interface



Atomic geometry retained

Candidate motifs



Local physical partitions

Predict and construct

Test interactions jointly
Test zone boundaries
Test collective response

Transfer across materials

Different motifs may act together; physical tests establish the grouping

Physical principles for Australia's quantum, advanced-manufacturing and energy ambitions. [1,2]

Which features must an interface preserve?

1 Identify the relevant interface

Does the model contain the interactions that cause the behaviour we want to understand?

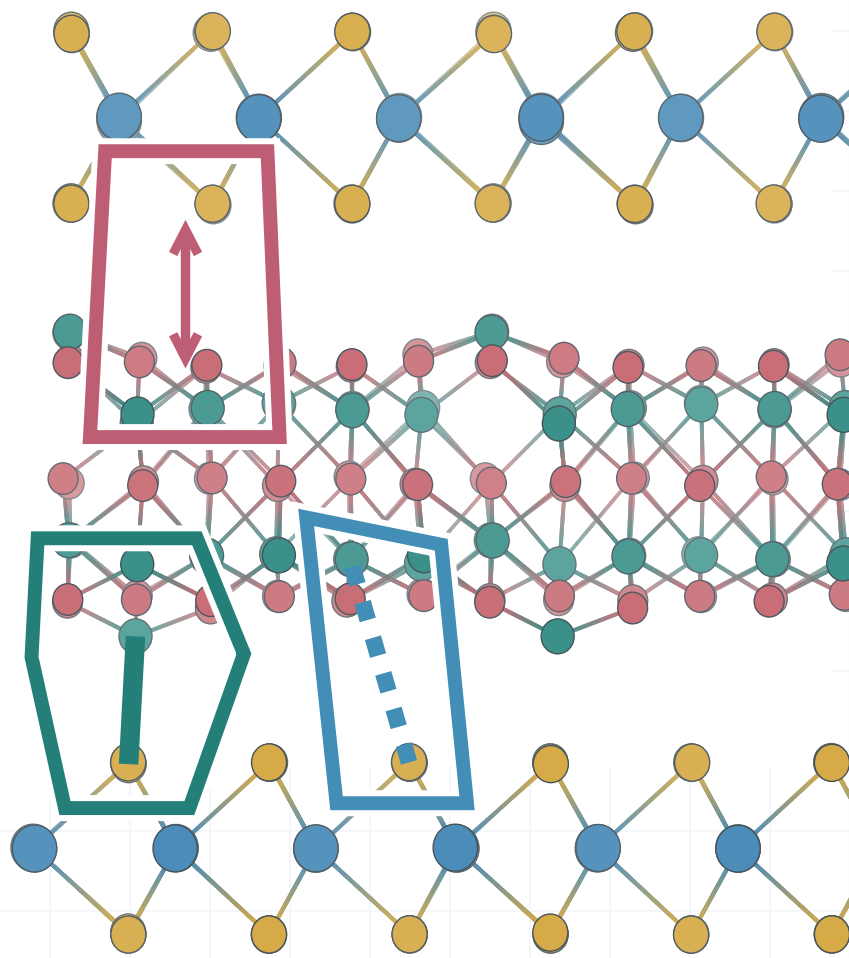
2 Construct the right environment

Can another physically stable interface retain those interactions and their useful response?

The hypothesis

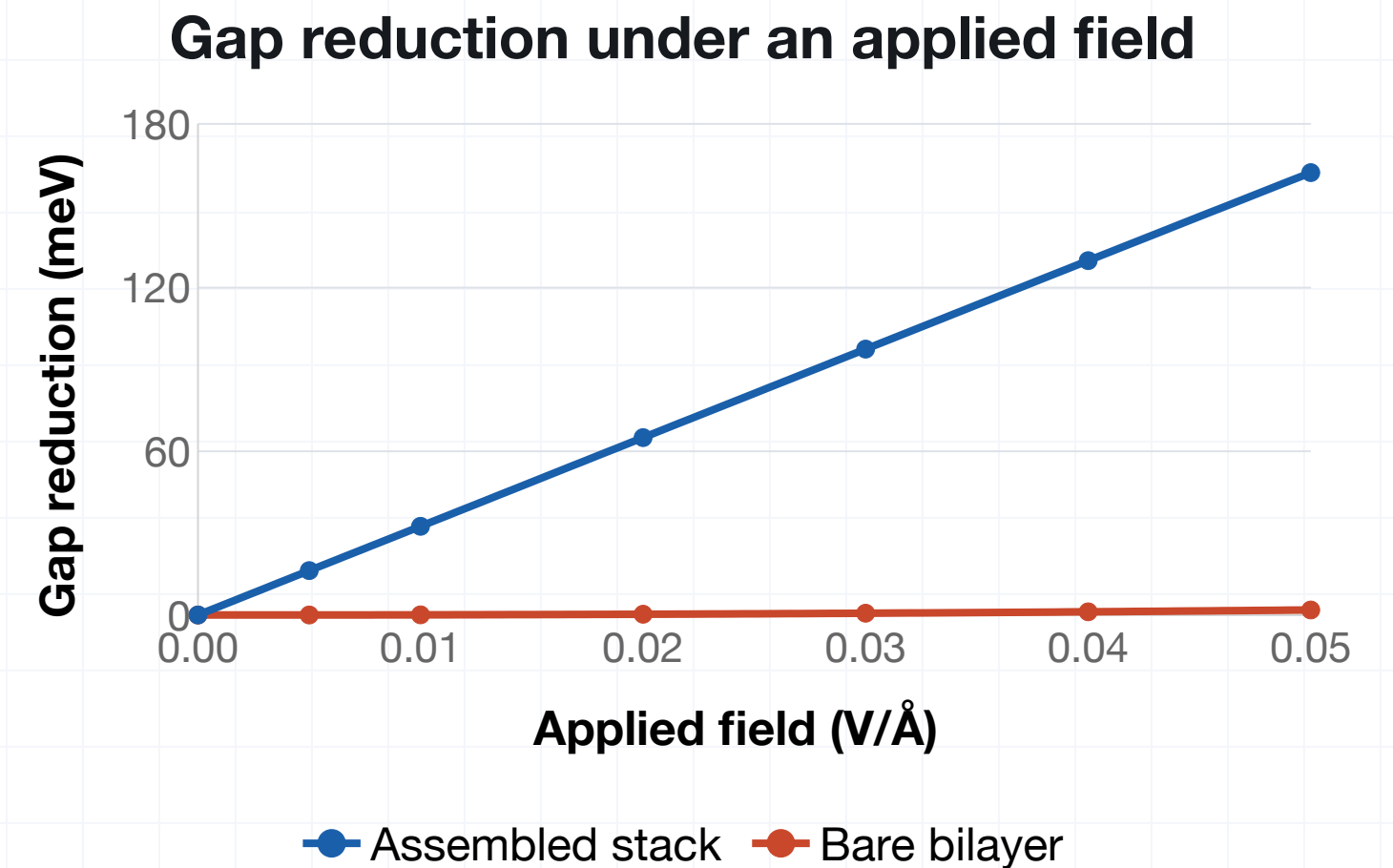
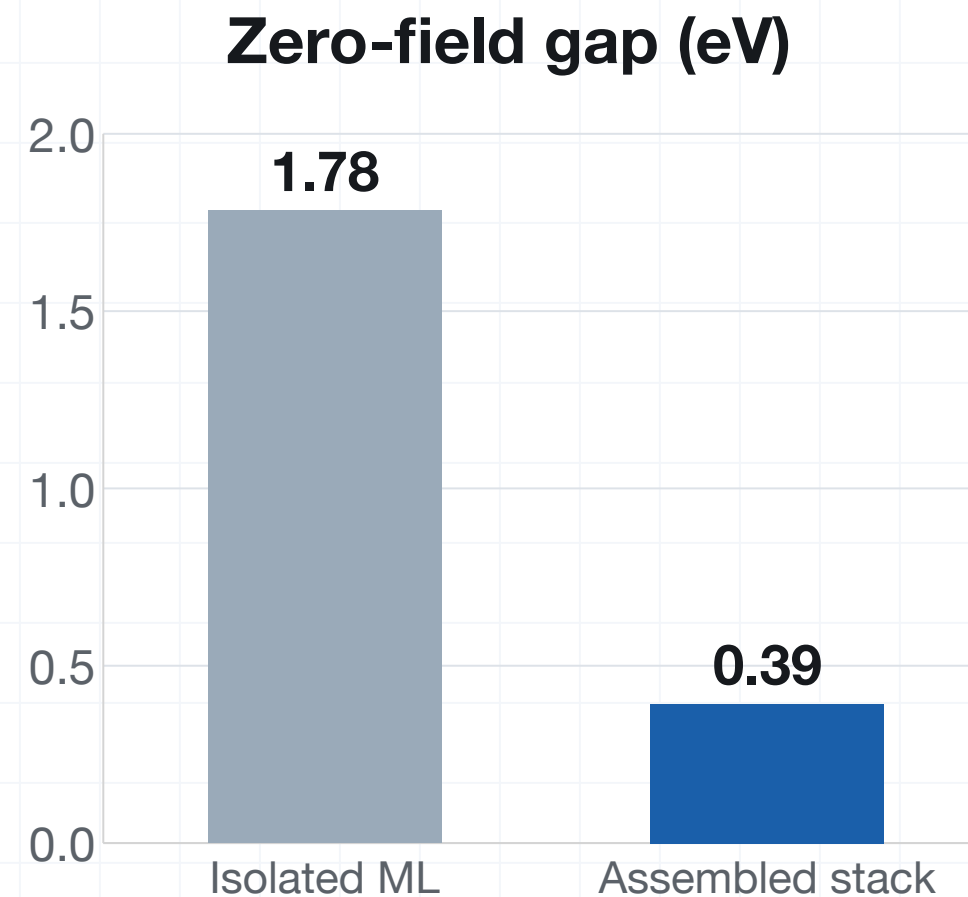
A compact group of interactions, with specified surroundings, can explain and reproduce a chosen interface response.

Complex interfaces can retain strong electrical control



MX_2 -oxides- MX_2

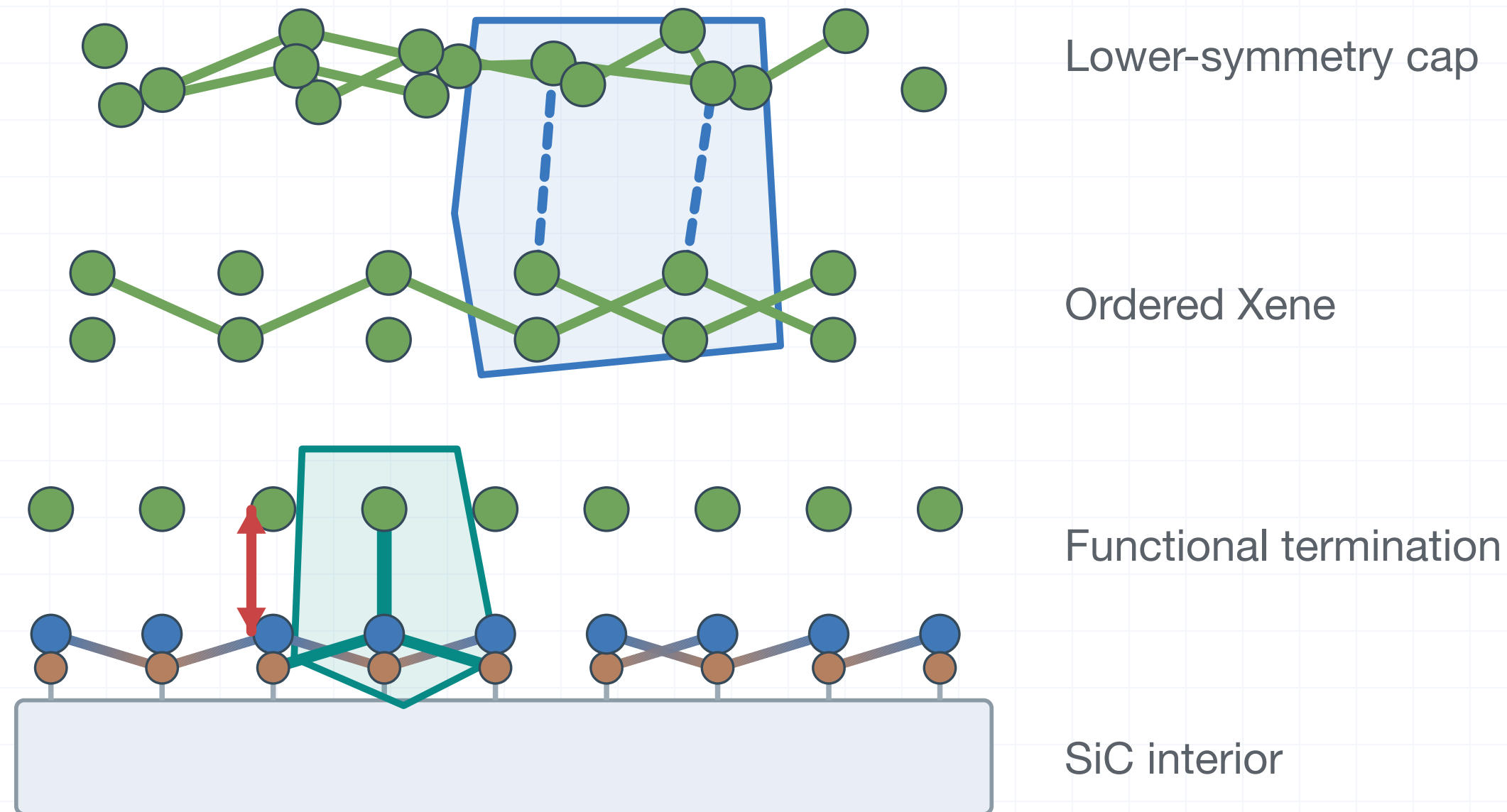
Candidate local environments



Electronic reconstruction need not destroy field sensitivity.

The Fellowship will separate charge redistribution, orbital mixing and screening.

An ordered layer may survive in less ordered surroundings



WHAT PROTECTS THE LAYER?

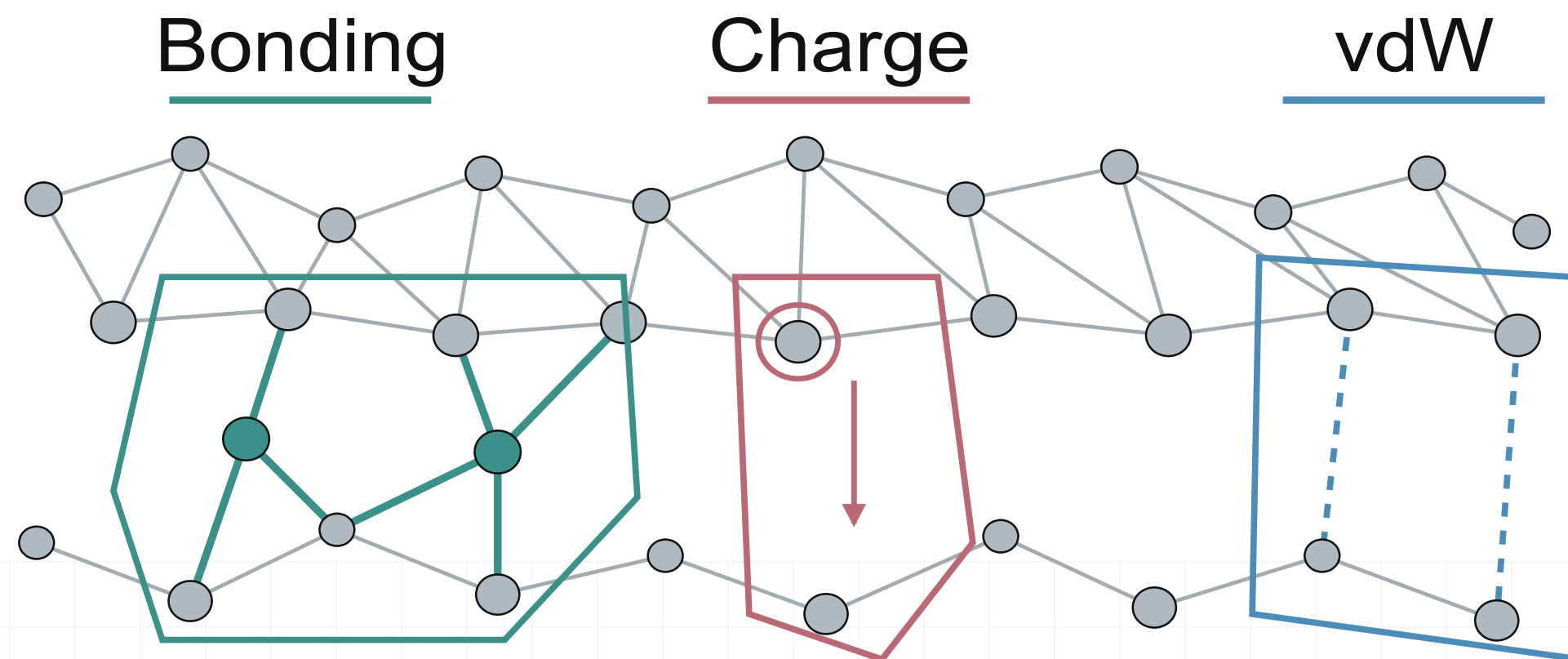
Passivation?
Confinement?
Their joint action?

Change the upper and lower environments separately, then together.

Illustrative reconstruction. Structural persistence and electronic function require separate tests.

Feature Zones test which interactions preserve function

A response-specific group of coupled atomic environments, with its boundary and environmental conditions established by tests.



A testable physical unit

Remove interactions to test necessity.
Recreate them to test sufficiency. Predict where the description succeeds or fails.

Graph methods propose groups. Controlled calculations establish their meaning.

Three work packages develop one physical explanation

WP1 Identify

Which interactions are necessary?

Remove or change interactions separately and jointly. Establish their reach and required surroundings.

WP2 Construct

Are those conditions sufficient?

Recreate interactions in relaxed alternatives. Test whether they reproduce the mechanism and response.

WP3 Generalise

Where does prediction hold?

Predict unseen material pairs. Quantify errors and failures as disorder and interface area change.

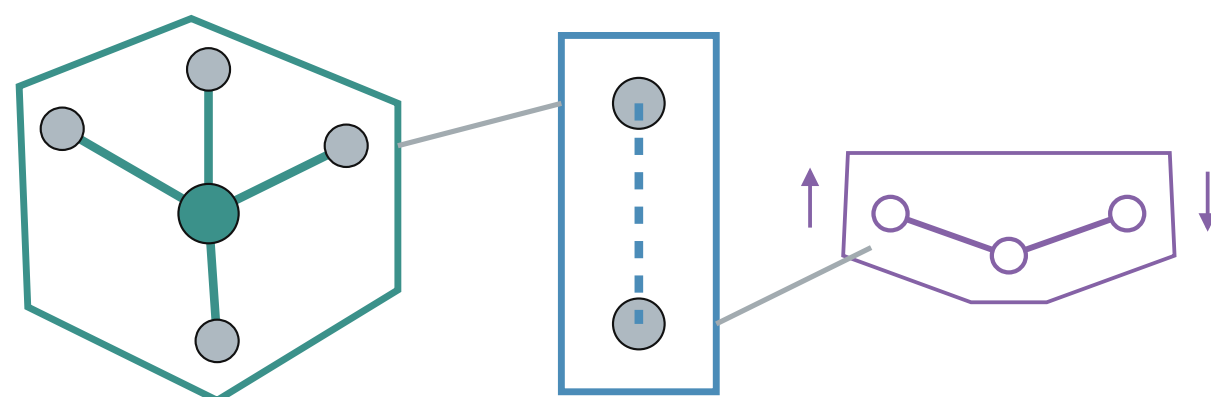
Structural persistence → useful electronic states

Electrical response → useful current flow

Both doctoral projects traverse all three packages. I lead the shared theory and decisive comparisons.

Does grouping add physical information?

Propose candidate motifs



Test interactions and grouping

- Bonding: charge and force
- vdW: separation and energy
- Exchange: ligand and spin states

Separate + joint tests; vary surroundings; compare full atomic graphs

Matched comparison

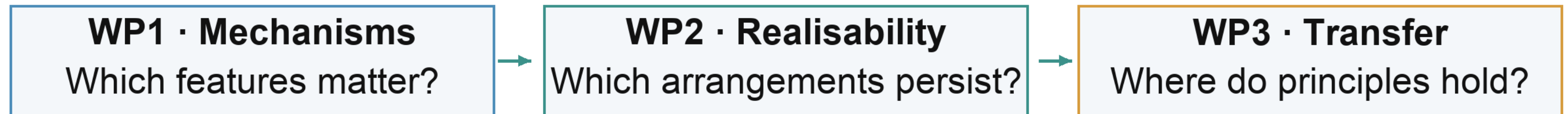
Compare grouped and ungrouped graphs with equal inputs and budgets. Remove group membership to isolate its contribution.

Independent transfer test

Reserve six material pairs and complete perturbation sequences. Predict before seeing their electronic results.

Tested interface principles and their predictive limits

From interface mechanisms to general physical principles



Matched comparisons · independent tests · explained failures

New understanding of robust electronic function

Materials physics: necessary and sufficient conditions

Computer science: tested representations and failure limits

Fabrication research: maps of tolerable interface variation

InterfaceHandler (InHand) shares the models and reproducible tests supporting these findings.

I connect atomic mechanisms with material function

Dr Yuefeng Yin

Surfaces, interfaces and atomic disorder

Detailed calculations

First-principles interpretation of local mechanisms and electronic states.

Efficient models

Electronic models that reach larger structures and transport.

Experimental connections

Physical explanations of observed material behaviour.

The Fellowship develops a new scientific question from this established modelling expertise.

Original modelling is tested through collaborative science

Established contribution	Evidence	What it enables here
Interfaces and quantum states	First-principles-to-localised models NJP (2021); MTP (2025)	Identify how surrounding layers reshape or preserve function.
Electrode interfaces and magnetic disorder	Transferred electrodes: ACS Nano (2025) Disordered magnetism: Matter (2025)	Test when imperfect structures retain useful behaviour.
Atomic dynamics and thermal transport	Theory linked with observed response Nature Communications (2026)	Connect mechanism tests with experimentally meaningful quantities.

My contribution is a physical explanation that can be examined, challenged and transferred.

I lead a funded programme in interface research

A\$650K

Total AEA Ignite project value
Lead Entrepreneur

674

Completed geometry–field
calculations across 36 stacks

Lead inventor

Pending international
patent application

**Careful interface design supported by agent-assisted coding
and high-throughput computational screening.**

Existing calculations provide evidence. New Fellowship tests establish sufficiency and transfer limits.

My research leadership and two complementary PhD projects

Yuefeng Yin · Chief Investigator

Develop the theory, design decisive tests, validate methods and integrate the findings.

PhD 1 · Quantum environments

Bismuthene integration and electronic states.

Ordered Xene / SiC probes structural persistence.

ARC stipend for four years.

A\$99,970 in research costs, alongside stipends. Monash cash support totals A\$235,180.

Both students identify, construct and test transfer. Shared methods connect two independent doctoral questions.

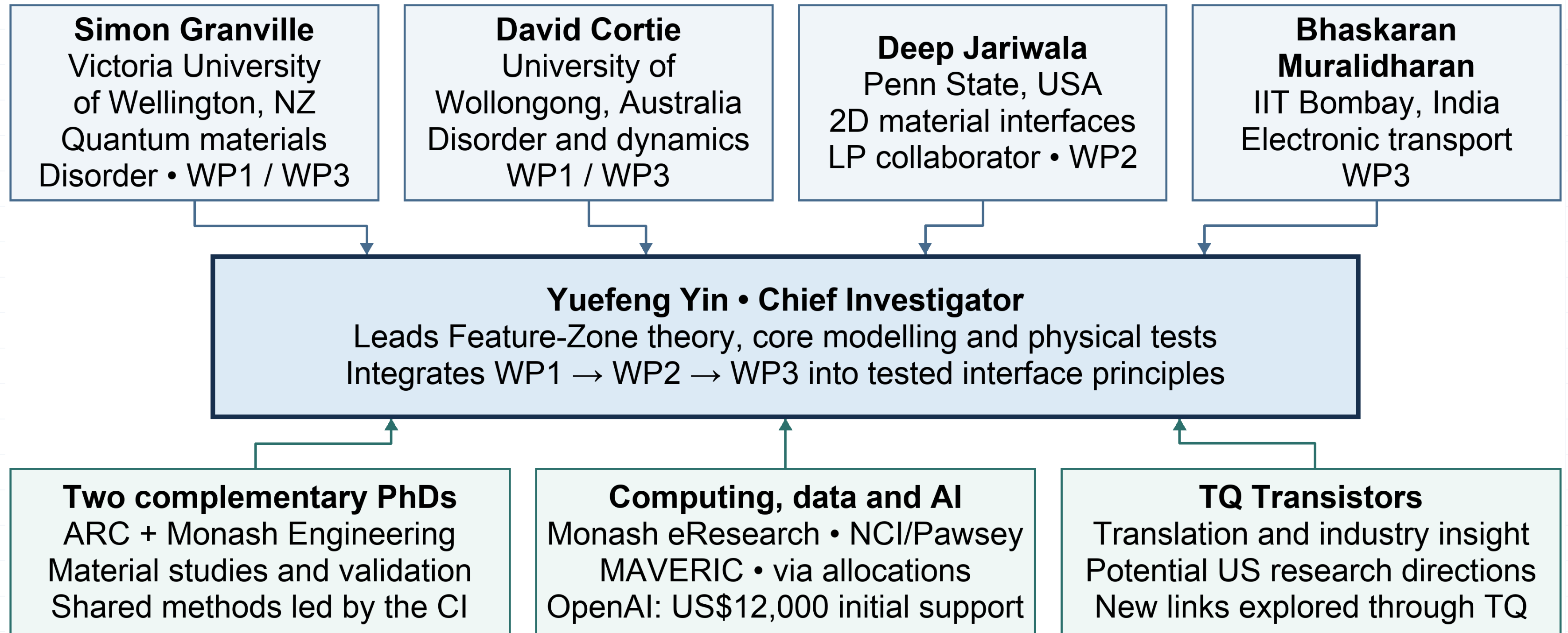
PhD 2 · Electronic contacts

Carrier injection and electrical control.

MX₂ stacks motivate tests of useful current flow.

Faculty strategic stipend for 3.5 years.

A focused network supports the research I lead



Understandable and reproducible interface function

Which interactions matter?

Which interfaces can realise them?

Where do those principles transfer?

**A scientific foundation for integrating quantum materials
and designing more energy-efficient electronics.**

Four-year research plan and doctoral progression

Activity	Year 1	Year 2	Year 3	Year 4
WP1 · Identify	M1: mechanisms	Refine boundaries	Test exceptions	Synthesis
WP2 · Construct	Pilot alternatives	M2: sufficiency	Test predictions	Design principles
WP3 · Generalise	Baseline tests	Plan held-out tests	M3: transfer limits	Independent tests
PhD 1 · ARC, 4 years	Methods and cases	Independent papers	Transfer studies	Thesis completion
PhD 2 · Faculty, 3.5 years	Methods and cases	Independent papers	Transfer studies	Complete in H1
CI leadership	Shared theory	Decisive tests	Cross-family tests	M4: synthesis

Six development pairs in WP2; six reserved pairs in WP3. Each PhD takes one family through all three packages.

The comparison is about explanatory value and transfer

Existing advance	What it helps establish	The further question
Compatibility screening	Which materials may match?	Which interactions create the response?
Structure generation	Which geometries are accessible?	Does the mechanism survive relaxation?
Learning from atomic images	Which local structures are present?	Which environments must act together?
Atomic graphs	Represent atoms and relationships	Does grouping improve compression or transfer?

Independent test sets exclude entire configurations and material pairs.

Testing where local descriptions succeed and fail

Uncertainty	Scientific response
Local zones omit essential physics	Establish the missing screening or coupling. Define the limit of a local description.
Constructed motifs relax away	Use the loss of function to determine physical realisability and constraints.
More complex learning adds little value	Use transparent descriptors and matched baselines. Escalate learning only with evidence.
Large calculations exceed affordable scope	Prioritise mechanisms and independent validation using staged computing allocations.

Existing AEA and Linkage programmes develop transistors. This Fellowship tests physical sufficiency and transfer.

Preliminary observations and the mechanisms still to test

Supported observation	Interpretation or test still needed
MX ₂ stack gap ≈ 0.392 eV Isolated monolayer ≈ 1.784 eV	Resolve charge redistribution, orbital mixing and screening.
At 0.01 V/Å: gap reduction Stack 32.497 meV; bare bilayer 0.057 meV	Separate field sensitivity from useful current injection. No stronger-binding claim without binding energies.
Ordered Xene layer in supplied structural figure	Reconstructed geometry is illustrative. Test relaxation, structural protection and electronic function independently.
674 geometry–field calculations / 36 stacks	This counts completed calculations, not 674 unique structures or a validated Feature-Zone benchmark.

Research costs and institutional support

A\$99,970

Other research expenditure over four years

Research expenditure	A\$
Travel and research exchanges	60,345
Equipment and VASP licence	21,625
Publication and dissemination	18,000
Total excluding salary and stipend	99,970

ARC request A\$1,022,634

Monash cash A\$235,180

Equipment across WP1–WP3

Mac Studio A\$11,445
Local models and shared research analysis

NAS A\$2,180
Active datasets and model checkpoints

VASP group licence A\$8,000

Project costs including the ARC PhD: Y1 \$59,963 · Y2 \$58,863 · Y3 \$59,408 · Y4 \$59,088

GST-exclusive. Final Mac Studio specification and VASP quote to confirm. Travel and publication costs are estimates.

Selected research underpinning the pitch

C1	Authors	Publication	Identifier
5	Y. Yin et al.	Materials Today Physics 59, 101897 (2025).	doi:10.1016/j.mtphys.2025.101897
7	Y. Yin et al.	ACS Nano 19, 3579–3588 (2025).	doi:10.1021/acsnano.4c13592
9	Y. Yin et al.	New Journal of Physics 23, 063042 (2021).	doi:10.1088/1367-2630/ac04c9
12	E. Gerber et al.	Nature Communications 14, 7921 (2023).	InterMatch
13	N. T. Taylor et al.	npj Computational Materials 11, 258 (2025).	RAFFLE
14	M. Ziatdinov et al.	Nature Machine Intelligence 4, 1101–1112 (2022).	AtomAI
15	A. Leitherer et al.	npj Computational Materials 9, 179 (2023).	AI-STEM
18	Y. Yin et al.	Matter 8, 101988 (2025).	doi:10.1016/j.matt.2025.101988
19	Y. Yin et al.	Nature Communications 17, 5267 (2026).	doi:10.1038/s41467-026-71754-9

Y. Yin et al. indicates first, co-first or corresponding authorship in this presentation.
[11] Preliminary calculations and unpublished manuscript; protected material labels used throughout.