AEA IGNITE PROGRESS REPORT

QUANTUM MATERIALS

Interface-first design of low-energy quantum devices

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Full report, data and list of author affiliations:
yyfforce.github.io

INTRODUCTION: Low-energy electronics — topological transistors, spin–orbit logic and negative-capacitance devices — are built by stacking dissimilar two-dimensional (2D) and thin-film materials. Whether a device concept survives depends less on the isolated material than on its interfaces: band alignment, orbital hybridisation, strain and disorder decide what actually reaches a working stack.

RATIONALE: Interface screening has so far been done one "hero" calculation at a time. We built **InterfaceHandler (InHand)**, an open-source package that automates lattice-matched supercell construction for arbitrary pairs of crystals, and coupled it to a high-throughput density-functional theory (DFT) workflow. The program targets three material families with established bulk physics — Heusler ferromagnetic films, 2D bismuth allotropes and topological pyrite-type OsX_2 — and asks which interfaces keep their useful properties once contacted.

RESULTS: At the mid-point, InHand has generated 4,812 candidate interfaces across the three families, of which 1,241 show type-I or type-II band alignment and 292 have been converged with plane-wave DFT. Five of eleven milestones are complete and two more are in progress. Heusler films retain their large Berry curvature in 71% of converged stacks, and a first labelled dataset has been curated for the machine-learning surrogate that will replace most brute-force calculations in the second half.

CONCLUSION: An interface-first workflow turns device-stack selection from a case-by-case effort into a searchable design space. The remaining twelve months focus on the pyrite family, a first surrogate model and handing the best stacks to our industry partner for fabrication. □

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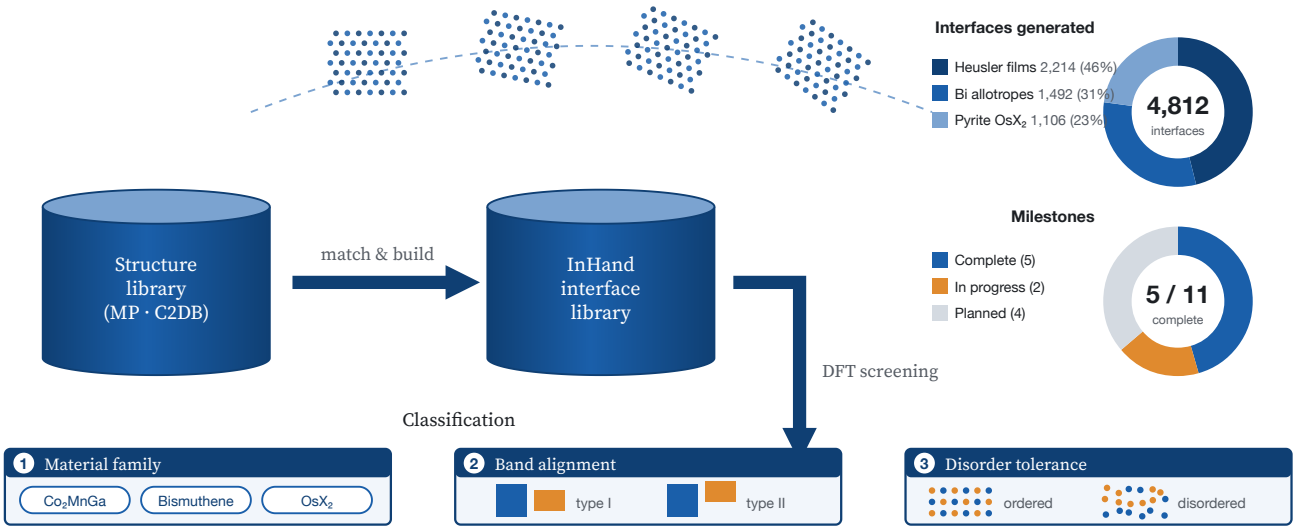

Workflow of the interface screening program. Candidate crystals from public structure databases are paired and lattice-matched by InHand to build an interface library, which is screened with DFT and classified by material family, band alignment and tolerance to disorder. Donuts show progress at the mid-term point (illustrative values).

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Interface-first design of low-energy quantum devices

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Heterostructure interfaces decide whether a promising quantum material becomes a working low-energy device, yet they are rarely screened systematically. This mid-term report describes an interface-first program built around InterfaceHandler (InHand), an open-source tool that constructs lattice-matched supercells and feeds them to high-throughput first-principles calculations. We summarise progress across three material families, report the screening statistics to date, and set out the plan, risks and deliverables for the second half of the project.

Two-dimensional materials and ultrathin films have opened a route to electronics that dissipates far less energy than silicon (*1–3*). Topological edge channels, large Berry curvature and spin–momentum locking all promise low-dissipation transport, but every one of these properties is defined for an idealised, isolated crystal (*4*, *5*). A real device places that crystal against a substrate, a gate dielectric and metallic contacts.

The physics at those contacts — charge transfer, hybridisation, strain and interfacial disorder — can switch a topological state off, pin the Fermi level or wash out the very signal a device relies on. Predicting it requires calculations on the interface itself, and the number of plausible interfaces grows combinatorially with the number of candidate materials, orientations and terminations.

This project replaces the "one hero calculation" approach with a systematic search. Its three streams are (i) software to generate interfaces automatically, (ii) high-throughput screening of three material families with density-functional theory (DFT), and (iii) machine-learning surrogates trained on the resulting data to extend the search at a fraction of the cost.

Interface construction with InHand

Given two bulk or 2D crystals, InHand enumerates supercells of each whose in-plane lattices coincide within a strain tolerance. For lattice vectors $\mathbf{a}_{1,2}$ (substrate) and $\mathbf{b}_{1,2}$ (overlayer), a match exists when integer matrices M and N satisfy

$$M\begin{pmatrix}\mathbf{a}_1\\ \mathbf{a}_2\end{pmatrix} \approx R(\theta)\,N\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\end{pmatrix}, \qquad |\,\varepsilon\,| < \varepsilon_{\max} \tag{1}$$

where $R(\theta)$ is an in-plane rotation and ε the residual strain applied to the overlayer. Candidate cells are ranked by strain, area and number of atoms so that the smallest physically faithful supercell is passed to DFT (Fig. 1).

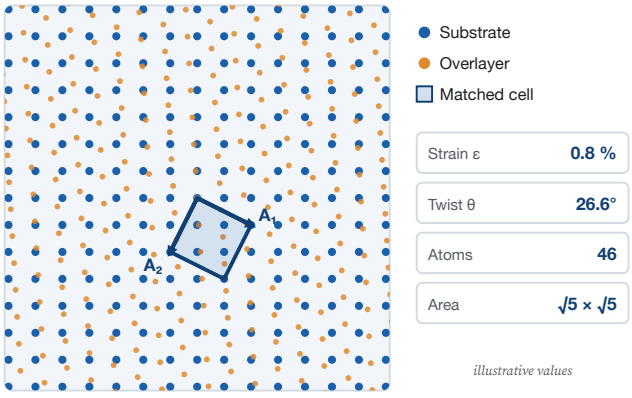

Fig. 1. Coincidence-lattice matching. A square substrate (blue) and a rotated hexagonal overlayer (orange) share a √5 × √5 supercell spanned by $\mathbf{A}_1$ and $\mathbf{A}_2$. InHand scores each candidate by residual strain, twist angle and cell size.

Version 2.1 of InHand completes Phase 1 of the software plan: structure import from public databases, the √n supercell search and automatic termination handling. Phase 2 adds a stable Python API for workflow engines and is on track for month 16.

Screening progress

All generated interfaces pass through the same three-stage screen: a fast band-alignment estimate from vacuum-aligned band edges, a relaxed low-precision DFT calculation, and a converged calculation with spin–orbit coupling for the survivors. Figure 2 shows the size of each stage per family.

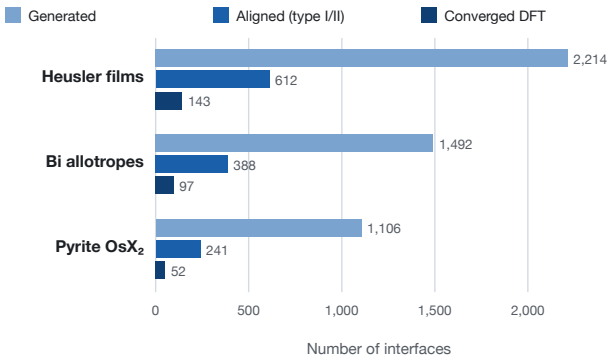

Fig. 2. Screening funnel by material family. Interfaces generated by InHand, those with type-I or type-II band alignment, and those converged with full DFT at the mid-term point (illustrative values).

Heusler ferromagnetic films

Co_2MnGa-type films were previously shown to retain a large Berry curvature even when fully disordered (*6*). Within the converged set, 71% of film/substrate stacks keep an anomalous Hall conductivity within 20% of the free-standing value; the failures cluster on substrates with strong Mn–O bonding.

2D bismuth allotropes

For bismuthene, the question is whether the topological edge state survives a realistic contact (*7*). Screening is 70% complete; early results favour van der Waals contacts with large work functions, which preserve the band inversion.

Prepared by Y. Yin · Department of Materials Science and Engineering, Monash University · 29 September 2026

KEY RESULT SO FAR

Disorder tolerance, not lattice mismatch, is the main filter: most interfaces that fail do so because interfacial disorder closes the gap or quenches the Berry curvature.

Timeline and milestones

The project runs for 24 months across three research streams and a translation activity. Figure 3 and Table 1 give the status of each milestone at month 12.

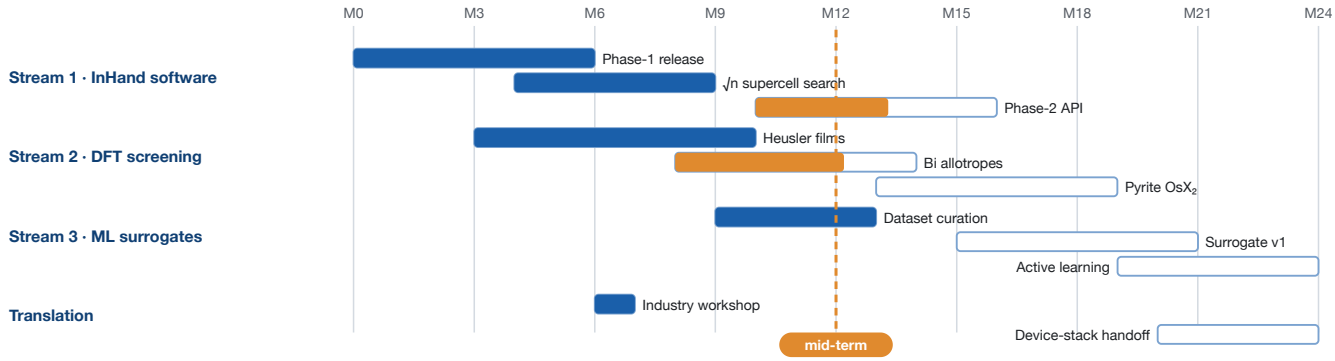

Fig. 3. Milestone timeline. Filled bars are complete (blue) or in progress (orange, filled to the fraction done); open bars are planned. The dashed line marks this report.

Table 1. Milestone status at the mid-term point.

Stream	Milestone	Due	Status
Software	InHand Phase-1 release	M6	**Complete**
Software	√n supercell search	M9	**Complete**
Software	Phase-2 Python API	M16	In progress (55%)
Screening	Heusler films	M10	**Complete**
Screening	Bi allotropes	M14	In progress (70%)
Screening	Pyrite OsX_2	M19	Planned
ML	Dataset curation	M13	**Complete**
ML	Surrogate model v1	M21	Planned
ML	Active-learning loop	M24	Planned
Translation	Industry workshop	M7	**Complete**
Translation	Device-stack handoff	M24	Planned

M = project month. Illustrative example.

Risks and plan for the second half

1. **Compute budget.** Converged spin–orbit calculations dominate cost; the surrogate model is designed to cut the number needed by roughly an order of magnitude.
2. **Pyrite family.** OsX_2 surfaces have several competing terminations; InHand's termination handling will be benchmarked on a small set first.
3. **Validation.** The top-ranked stacks will be shared with experimental collaborators and our industry partner for growth and transport tests.

The second half shifts effort from building tools to using them, ending in a ranked shortlist of device stacks.

Methods

Interfaces were generated with InHand v2.1 using a strain tolerance of 2% and a maximum of 120 atoms per cell. Electronic structures were computed with the Vienna *ab initio* simulation package (*8*) using the projector augmented-wave method (*9*) and the PBE functional; converged calculations include spin–orbit coupling and van der Waals corrections. Band alignments were estimated from vacuum-aligned band edges. Calculations ran on NCI Gadi.

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SUPPLEMENTARY MATERIALS

Full interface library, screening tables and convergence tests are available on request.

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