

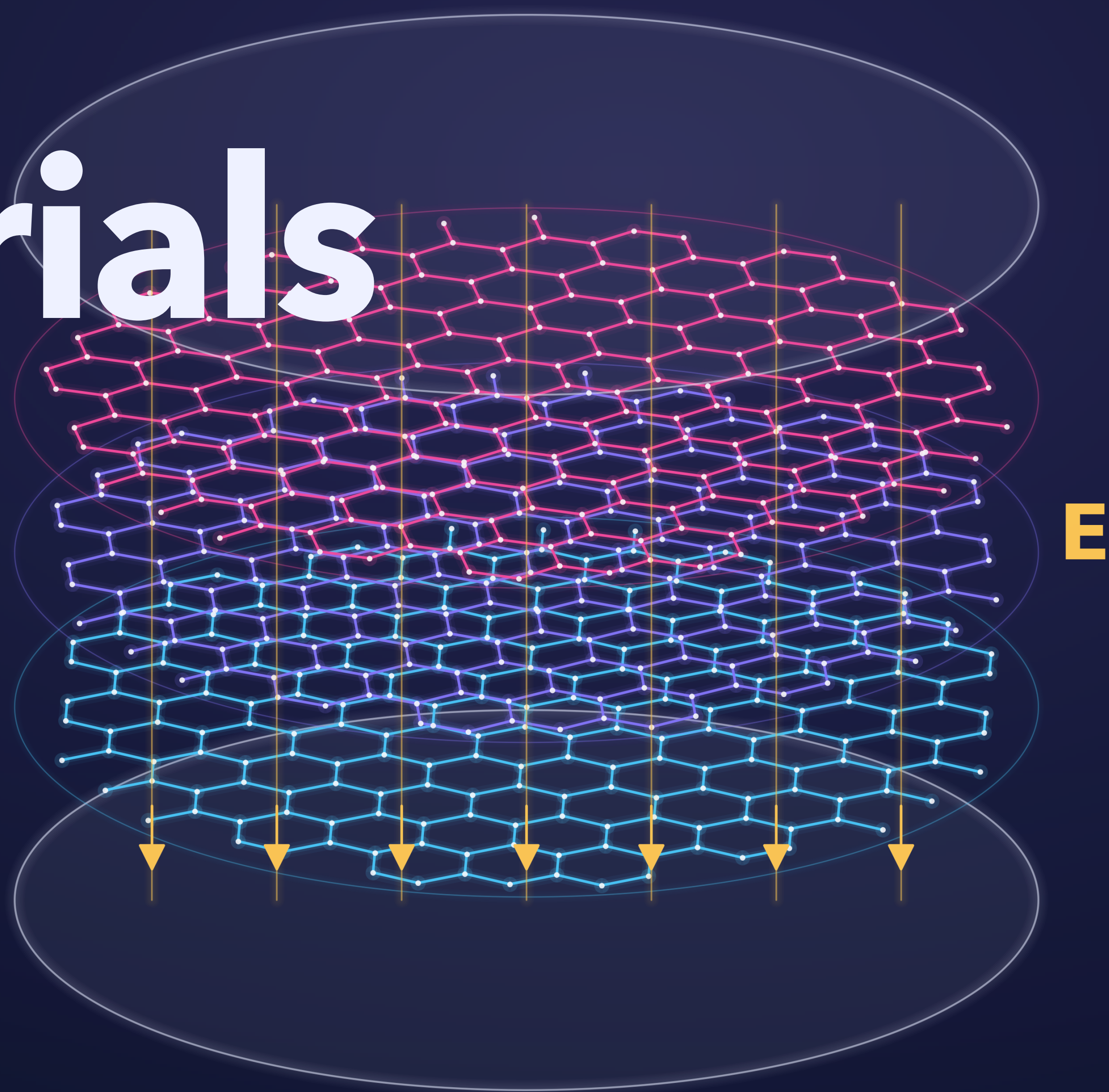
HONOURS PROJECTS

Reconfigurable Quantum Materials by Design

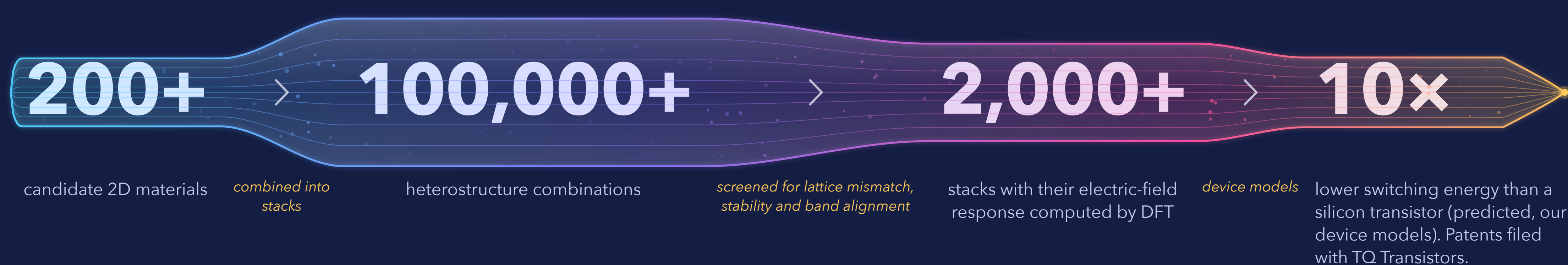
Theory · Computation · AI · Supercomputers

From atoms and Hamiltonians to devices: designing tunable quantum materials that make a real difference.

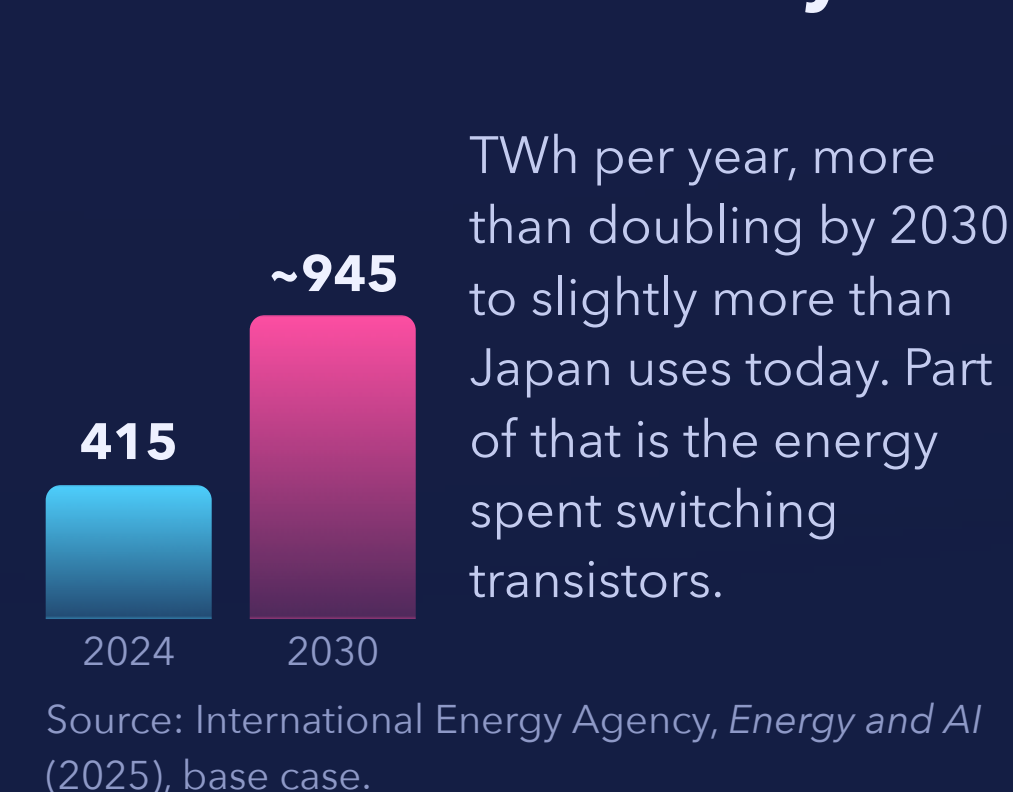
We compute how electrons in 2D materials respond to an electric field, a twist between layers or magnetic order, and use the results to design materials and devices with experimental groups in this School.



Our screen of stacked 2D materials

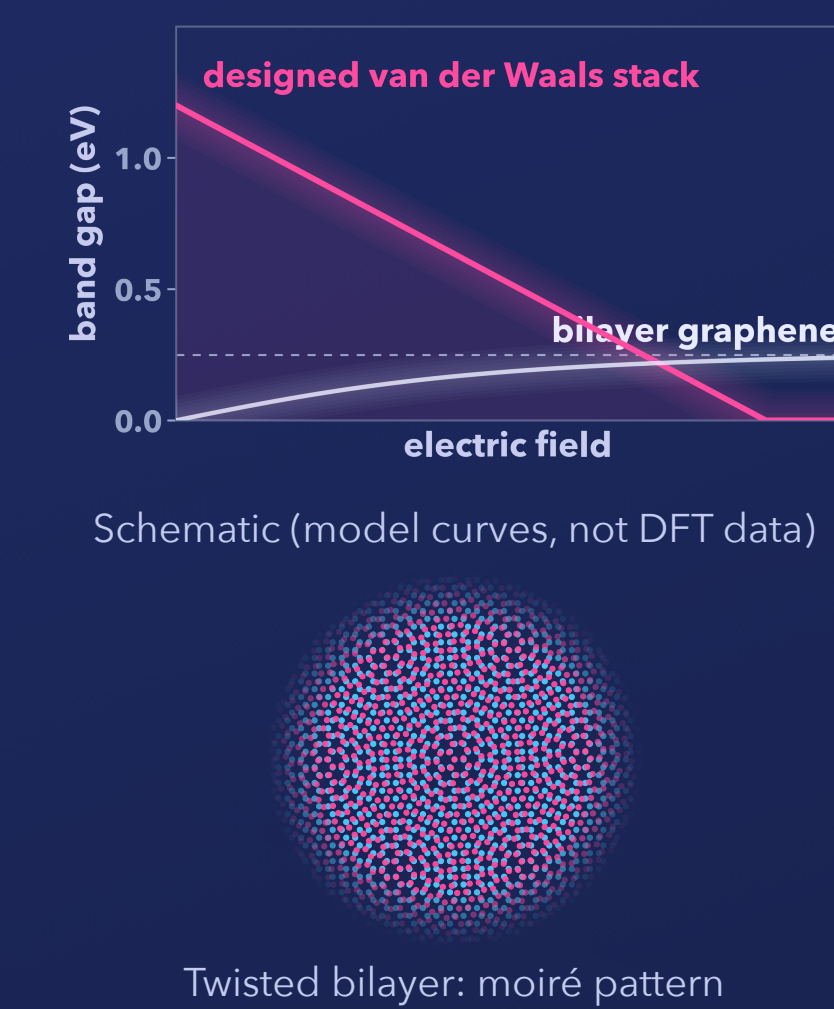


Data-centre electricity use



Projects

Two places available.



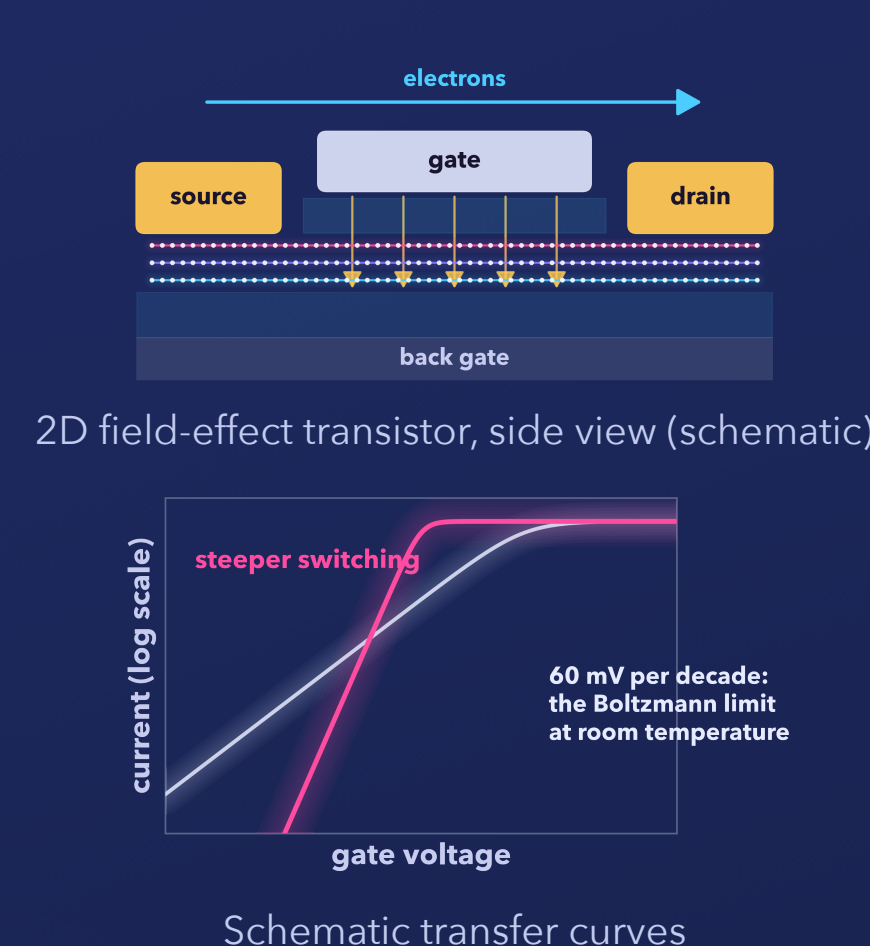
PROJECT 1

Field-tunable electronic structure of stacked and twisted (moiré) 2D materials

with Prof Michael Fuhrer

Bilayer graphene opens a band gap under a perpendicular electric field, but it saturates at about 250 meV. Our high-throughput DFT screen has found van der Waals stacks whose gap starts above 1 eV and closes steadily with field instead of saturating. You will build the minimal model that explains both and test it against our data on 2,000+ stacks, then extend it to twisted (moiré) bilayers with tight binding.

Wang *et al.*, *Mater. Today Phys.* **59**, 101897 (2025) · Yin *et al.*, *Mater. Today Phys.* **36**, 101168 (2023)



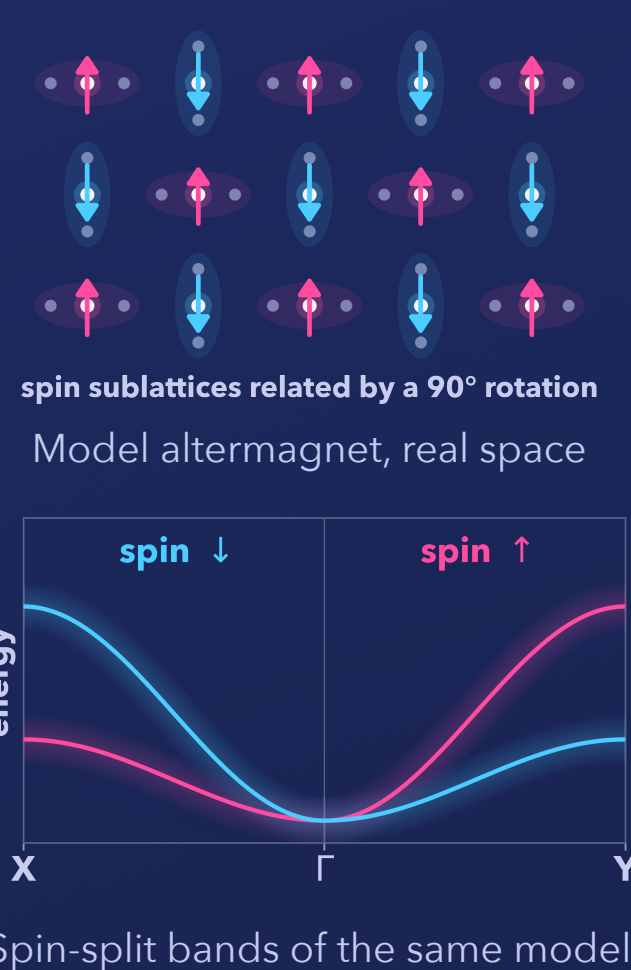
PROJECT 2

Large-scale quantum transport models of 2D field-effect devices

with Prof Michael Fuhrer

A conventional transistor cannot switch more steeply than 60 mV per decade at room temperature. A channel driven through a topological transition by a gate field could beat that limit (Prof Fuhrer's negative-capacitance topological quantum FET), but showing it needs channel, contacts and gate electrostatics in one self-consistent calculation. You will build the transport models (NEGF), first in Kwant, then on GPUs, for devices made in his lab.

Fuhrer *et al.*, *IEEE IEDM*, 38.2.1-38.2.4 (2021) · Yin *et al.*, *npj Quantum Mater.* **4**, 47 (2019)

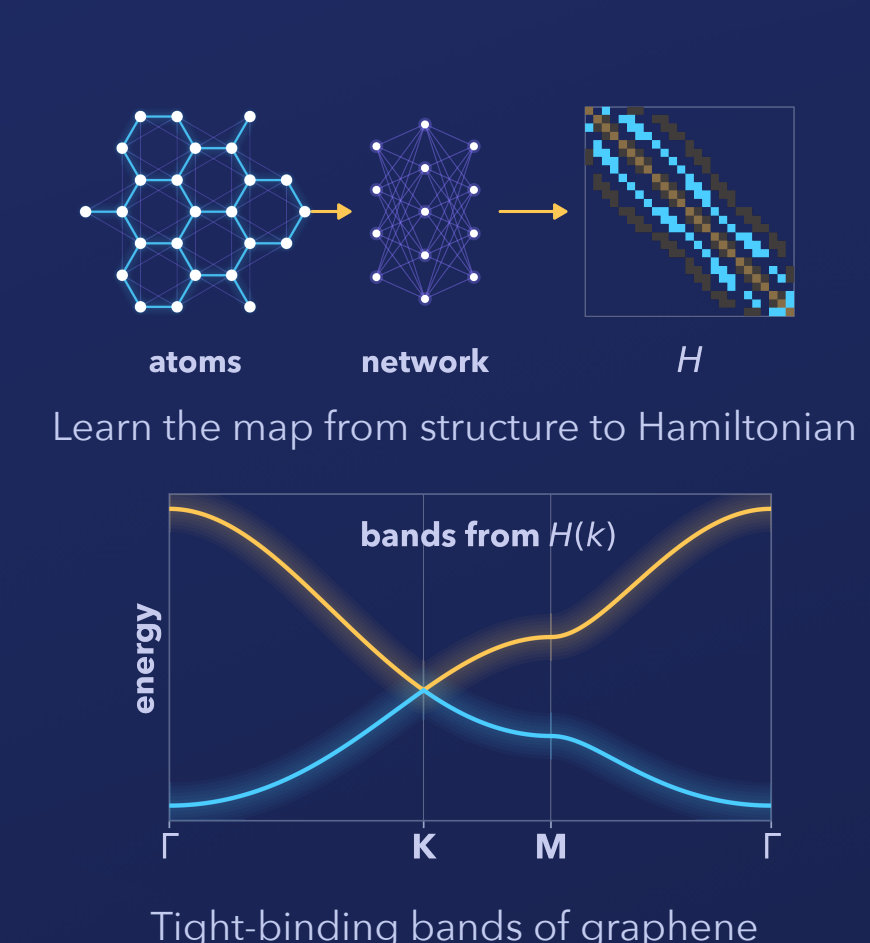


PROJECT 3

d-wave spin splitting in two-dimensional altermagnets

Altermagnets are collinear magnets with zero net magnetisation whose bands are nonetheless spin split, without spin-orbit coupling, in a d-wave or higher even-parity pattern set by crystal symmetry. Our recent work on 2D altermagnets whose d-wave splitting is locked to their electric polarisation is the starting point. You will use symmetry analysis, DFT and a minimal band model to find 2D altermagnets with large spin splitting.

Liu & Medhekar, *Nano Lett.* **25**, 13411 (2025) · Liu *et al.*, *Nano Lett.* **24**, 11295 (2024) · Zhao *et al.*, *Adv. Sci.* **e76833** (2026)



PROJECT 4

Machine-learned Hamiltonians for 2D stacks too large for DFT

DFT gives the Hamiltonian of a 2D material in a local-orbital basis, at a cost that grows as the cube of the atom count, so twisted and multilayer stacks with thousands of atoms are out of reach. You will train graph neural networks (the DeepH approach) to predict that Hamiltonian from the atomic structure alone, test them against DFT, and feed the band structures of large stacks into the transport models of Project 2.

Background: Li *et al.*, *Nat. Comput. Sci.* **2**, 367 (2022) · Gong *et al.*, *Nat. Commun.* **14**, 2848 (2023)

Approaches

Python JAX PyTorch VASP Wannier90 Kwant tight binding ML-potentials (MACE) learned Hamiltonians

Calculations run on the national supercomputers (NCI Gadi, Pawsey Setonix) and on Monash's NVIDIA Blackwell AI system. We write code with AI coding agents.



Setonix, Pawsey Supercomputing Research Centre. Artwork: Margaret Whitehurst.

Who we're looking for (any one is enough)

- Third-year quantum mechanics and some condensed matter
- Some coding. No DFT experience needed
- Comfort with Hamiltonians, symmetry and linear algebra
- An interest in physics that ends up in a device

Open to

• Honours

• Masters

• PHS2350/3350 projects

• PhD after honours

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Come and talk to me, or email any time

Prof Nikhil Medhekar

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Research profile