

References

Project title	InterfaceHandler: Complex Interface for Semiconductors
Lead CI	Dr Yuefeng Yin — Department of Materials Science and Engineering, Monash University

Methods, software and workflow references

- [1] G. Kresse, J. Furthmüller. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Physical Review B* 54, 11169 (1996).
- [2] G. Kresse, D. Joubert. From ultrasoft pseudopotentials to the projector augmented-wave method. *Physical Review B* 59, 1758 (1999).
- [3] J. P. Perdew, K. Burke, M. Ernzerhof. Generalized Gradient Approximation Made Simple. *Physical Review Letters* 77, 3865 (1996).
- [4] S. P. Ong, W. D. Richards, A. Jain, *et al.* Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. *Computational Materials Science* 68, 314–319 (2013).
- [5] A. H. Larsen, J. J. Mortensen, J. Blomqvist, *et al.* The atomic simulation environment — a Python library for working with atoms. *Journal of Physics: Condensed Matter* 29, 273002 (2017).
- [6] A. Jain, S. P. Ong, G. Hautier, *et al.* Commentary: The Materials Project — a materials genome approach to accelerating materials innovation. *APL Materials* 1, 011002 (2013).
- [7] K. Mathew, J. H. Montoya, A. Faghaninia, *et al.* Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. *Computational Materials Science* 139, 140–152 (2017).

Prior work supporting research track record and computational feasibility

- [8] W. Zhao, Y. Zhang, Y. Yin, *et al.* Giant Berry curvature in the amorphous ferromagnet Co₂MnGa. *Matter* 8, 101988 (2025).
- [9] C. Wang, Y. Yin, T. T. Huynh, M. S. Fuhrer, N. V. Medhekar. Edge-state stabilization and control in 2D topological crystalline insulators. *Materials Today Physics* 59, 101897 (2025).
- [10] Y. Yin, C. Wang, M. S. Fuhrer, N. V. Medhekar. Extracting unconventional spin texture in the 2D topological crystalline insulator bismuthene via tuning bulk–edge interactions. *Materials Today Physics* 36, 101168 (2023).
- [11] Q. Li, J. S. Smith, Y. Yin, C. Wang, M. V. Klymenko, J. H. Cole, N. V. Medhekar. Localized Wannier-function-based tight-binding models for 2D allotropes of bismuth. *New Journal of Physics* 23, 063403 (2021).
- [12] Y. Yin, M. S. Fuhrer, N. V. Medhekar. Selective control of surface spin current in topological pyrite-type OsX₂ (X = Se, Te) crystals. *npj Quantum Materials* 4, 47 (2019).