Yuefeng Yin

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Yuefeng Yin

Education

Mar 2012 – May 2016 **Ph.D. in Materials Science and Engineering**
Monash University
Melbourne, Australia
Thesis title: Tailoring the Electronic Structure of Graphene via Molecular Adsorption

Sep 2007 – Dec 2011 **B.Eng. (First Class Honours) in Materials Engineering**
Monash University(AU)/Central South University (CN)
Melbourne, Australia/Changsha, China
Thesis title: Molecular Dynamics Simulation of Graphene and Related Materials

Experience

Research

May 2017 - Current **Research Fellow** *Monash University,* Melbourne, Australia
Conducting research in topological materials under ARC Centre of Excellence in Future Low-Energy Electronic Technologies (FLEET).

May 2016 - Dec 2016 **Research Associate** *Monash University,* Melbourne, Australia
Conduct research on properties of PEG-based hydrogels using Monte Carlo Simulations.

Teaching and Visiting

May 2017 and May 2018 **Visiting Lecturer** *Central South University,* Changsha, China
Teach an undergraduate course on computational materials science as a part of Monash+CSU collaboration program.

Referees

Nikhil V. Medhekar Professor, Department of Materials Science and Engineering, Monash University, Australia, nikhil.medhekar@monash.edu

Michael S. Fuhrer Professor, Director of FLEET, School of Physics and Astronomy, Monash University, Australia, michael.fuhrer@monash.edu

Research Projects

2021 - Current **Developing DFT-Tight Binding Workflows for Topological Physics** *FLEET, Monash University*

Methodology/Codes applied: *Fortran/Python/VASP/Wannier90*

- The Nobel Prize-winning discovery of topological materials promises super-fast electron transport, revolutionizing electronics and suggesting potential for reduced energy consumption.
- In this project, I used advanced modeling techniques, including DFT and tight-binding methods, to create a simple approach for understanding the electronic properties of topological materials. This methodology not only deepens our understanding of these materials but also offers crucial insights for material designers and industrial partners, facilitating the accelerated development of innovative devices.

2017 - Current **Discovering New Topological Materials For Spintronics** *FLEET, Monash University*

Methodology/Codes applied: *Fortran/Python/MATLAB/VASP/Wannier90*

- Topological materials often derive inspiration from existing compounds rather than being entirely "new." Computational materials science efficiently screens material properties, aiding in the identification of those displaying topologically protected electronic features and playing a crucial role in predicting material behaviors.
- In this project, I discovered a Osmium-based pyrite compound as a topological material, revealing highly orientation-dependent spin transport behavior. This marks the first demonstration of such behavior in non-magnetic materials, highlighting the exciting potential of topological materials for pure spin transport and revolutionizing information transmission.
- I have also expanded the computational approach to unveil exotic transport behavior in two-dimensional magnetic thin films, establishing strong collaborations with experimentalists. Theoretical calculations not only explained observed phenomena but also provided valuable guidance for future experimental designs.

2012 - 2017 **Change Graphene For Better Electronics** *Medhekar Group, Monash University*

Methodology/Codes applied: *Python/MATLAB/VASP*

- Graphene, renowned for its simple honeycomb structure and remarkable properties, stands as a revolutionary material poised to reshape our future.
- In this project, I employed atomic simulations to explore the potential applications of graphene in electronic devices, with a focus on transistors. An important aspect of my work was introducing the weak interaction of alien molecules to graphene sheets, aiming to enhance graphene's functionality.
- I have established a fundamental understanding of the interaction between graphene and DNA/RNA nucleobases. This pioneering study offers indispensable insights into utilizing graphene for molecular sensing and applications, including DNA sequencing.

2012 - Current **2D Materials Beyond Graphene** *Medhekar Group, Monash University*

Methodology/Codes applied: *VASP/Wannier90*

- Computational materials science provides a distinct advantage, enabling the seamless application of methodologies across diverse materials, particularly valuable in nanotechnology.
- My research focuses on utilizing first principles calculations and tight-binding approaches to investigate the electronic, mechanical, and optical properties of various two-dimensional materials, such as MoS2, h-BN, and Kagome layers. The outcomes of these investigations have enriched our understanding of low-dimensional materials science beyond graphene, revealing their potential applications across a spectrum of fields.

Publication Summary

I have published 31 high-quality refereed journal articles, including theory-focused papers published in acclaimed journals such as Materials Today Physics (IF = 11.5), ACS Nano (IF = 17.1), npj Quantum Materials (IF = 5.7) and Journal of Physical Chemistry Letters (IF = 5.7). I also have published collaboration paper with significant computational contributions appearing in Nature Communications (IF = 16.6), Advanced Functional Materials (IF = 19.0) and Nano Letters (IF = 10.8). My publications have received 638 citations with an h-index of 15.

List of Publications

Research topic summary (selected papers):

- Electronic/spintronic structure of quantum materials: 3, 5, 10, 14, 16, 23.
- Changing graphene for better electronic materials: 2, 15, 20, 27, 30, 31.
- Exploring new approaches of materials modeling: 5, 14, 23.

Contribution summary (selected papers):

- First-authored paper / co-first-authored paper / paper as a corresponding author: 5, 9, 10, 14, 16, 17, 23, 26, 27, 30.
- Co-authored paper with significant original theoretical contributions by myself: 2, 4, 13, 15, 18, 20, 22, 25, 28, 29.
- Co-authored paper by supervising graduate students: 6, 7, 8, 21.

Publications by year:

1. Hong, Y., Deng, J., Kong, Q., Yin, Y., Ding, X., Sun, J., Liu, J.Z., Origin of different piezoelectric responses in elemental Sb and Bi monolayers, Physical Review B, 2024, 109, 35204.
2. Grubišić-Čabo, A., Kotsakidis, J.C., Yin, Y., Tadich, A., Haldon, M., Solari, S., Riley, J., Huwald, E., Daniels, K.M., Myers-Ward, R.L., Edmonds, M.T., Medhekar, N., Gaskill, D.K., Fuhrer, M.S., Quasi-free-standing AA-stacked bilayer graphene induced by calcium intercalation of the graphene-silicon carbide interface, Frontiers in Nanotechnology, 2023, 5, 1333127.
3. Mallett, B., Zhang, Y., Pot, C., Van Koughnet, K., Stanley, B., Buckley, R.G., Koo, A., Yin, Y., Medhekar, N.V., Granville, S., Using optical spectroscopy to probe the impact of atomic disorder on the Heusler alloy Co_2MnGa, Physical Review Materials, 2023, 7, 94203.
4. Aoki, M., Yin, Y., Granville, S., Zhang, Y., Medhekar, N.V., Leiva, L., Ohshima, R., Ando, Y., Shiraishi, M., Gigantic Anisotropy of Self-Induced Spin-Orbit Torque in Weyl Ferromagnet Co2MnGa, Nano Letters, 2023, 23, 6951-6957.
5. Yin, Y., Wang, C., Fuhrer, M.S., Medhekar, N.V., Extracting unconventional spin texture in two dimensional topological crystalline insulator bismuthene via tuning bulk-edge interactions, Materials Today Physics, 2023, 36, 101168.

6. Tang, L., Mao, Z., Wang, C., Fu, Q., Wang, C., Zhang, Y., Shen, J., Yin, Y., Shen, B., Tan, D., Li, Q., Wang, Y., Medhekar, N.V., Wu, J., Yuan, H., Li, Y., Fuhrer, M.S., Zheng, C., Giant piezoresistivity in a van der Waals material induced by intralayer atomic motions, Nature Communications, 2023, 14, 1519.
7. Jawa, H., Varghese, A., Ghosh, S., Sahoo, S., Yin, Y., Medhekar, N.V., Lodha, S., Wavelength-controlled photocurrent polarity switching in BP-MoS_2 heterostructure, Advanced Functional Materials, 2022, 32, 2112696.
8. Ghosh, S., Varghese, A., Jawa, H., Yin, Y., Medhekar, N.V., Lodha, S., Polarity-tunable photocurrent through band alignment engineering in a high-speed $WSe_2/SnSe_2$ diode with large negative responsivity, ACS Nano, 2022, 16, 4578-4587.
9. Varghese, A., Yin, Y., Wang, M., Lodha, S., Medhekar, N.V., Near-Infrared and Visible-Range Optoelectronics in 2D Hybrid Perovskite/Transition Metal Dichalcogenide Heterostructures, Advanced Materials Interfaces, 2022, 9, 2102174.
10. Trang, C.X., Li, Q., Yin, Y., Hwang, J., Akhgar, G., Di Bernardo, I., Grubisic-Cabo, A., Tadich, A., Fuhrer, Mo, S.-K., Medhekar, N.V., M.S., Edmonds, M.T., Crossover from 2D ferromagnetic insulator to wide band gap quantum anomalous Hall insulator in ultrathin $MnBi_2Te_4$, ACS Nano, 2021, 15, 13444-13452.
11. Fuhrer, M.S., Edmonds, M.T., Culcer, D., Nadeem, M., Wang, X., Medhekar, N., Yin, Y., Cole, J.H., Proposal for a negative capacitance topological quantum field-effect transistor, 2021 IEEE International Electron Devices Meeting (IEDM), 2021, 38.2.1-38.2.4.
12. Kumar, D., Hellerstedt, J., Field, B., Lowe, B., Yin, Y., Medhekar, N.V., Schiffrin, A., Manifestation of strongly correlated electrons in a 2D kagome metal–organic framework, Advanced Functional Materials, 2021, 31, 2106474.
13. Shivananju, B.N., Zhou, L., Yin, Y., Yu, W., Shabbir, B., Mu, H., Bao, X., Zhang, Y., Tian, S., Ou, Q., Li, S., Hossain, M.M., Zhang, Y., Shao, H., Xing, G., Medhekar, N.V., Li, C.-M., Liu, J., Bao, Q., Probing the dynamic structural changes of DNA using ultrafast laser pulse in graphene-based optofluidic device, InfoMat, 2021, 3, 316-326.
14. Li, Q., Smith, J.S., Yin, Y., Wang, C., Klymenko, M.V., Cole, J.H., Medhekar, N.V., Localized Wannier function based tight-binding models for two-dimensional allotropes of bismuth, New Journal of Physics, 2021, 23, 63042.
15. Grubišić-Čabo, A., Kotsakidis, J.C., Yin, Y., Tadich, A., Haldon, M., Solari, S., Di Bernardo, I., Daniels, K.M., Riley, J., Huwald, E., Edmonds, M.T., Myers-Ward, R., Medhekar, N.V., Gaskill, D.K., Fuhrer, M.S., Magnesium-intercalated graphene on SiC: Highly n-doped air-stable bilayer graphene at extreme displacement fields, Applied Surface Science, 2021, 541, 148612.
16. Zhang, Y., Yin, Y., Dubuis, G., Butler, T., Medhekar, N.V., Granville, S., Berry curvature origin of the thickness-dependent anomalous Hall effect in a ferromagnetic Weyl semimetal, npj Quantum Materials, 2021, 6, 17.
17. Qi, J., Yin, Y., Ding, X., Sun, J., Deng, J., Firstprinciples study of mechanical and optical properties for ZnS1xOx alloying compounds, Materials Today Communications, 2020, 24, 101259.
18. Wu, Y., Ou, Q., Yin, Y., Li, Y., Ma, W., Yu, W., Liu, G., Cui, X., Bao, X., Duan, J., Alvarez-Perez, G., Dai, Z., Shabbir, B., Medhekar, N., Li, X., Li, C.-M., Alonso-Gonzalez, P., Bao, Q., Chemical switching of low-loss phonon polaritons in αMoO_3 by hydrogen intercalation, Nature communications, 2020, 11, 2646.
19. Ye, H., Zhang, Y., Wei, A., Han, D., Liu, Y., Liu, W., Yin, Y., Wang, M., Intrinsic-strain-induced curling of free-standing two-dimensional Janus MoSSe quantum dots, Applied Surface Science, 2020, 519, 146251.

20. Kotsakidis, J.C., Grubišić-Čabo, A., Yin, Y., Tadich, A., Myers-Ward, R.L., DeJarld, M., Pavunny, S.P., Currie, M., Daniels, K.M., Liu, C., Edmonds, M.T., Medhekar, N.V., Gaskill, D.G., Vazquez de Parga, A.L., Fuhrer, M.S., Freestanding n-doped graphene via intercalation of calcium and magnesium into the buffer layer–SiC (0001) interface, Chemistry of Materials, 2020, 32, 6464-6482.
21. Collins, J.L., Wang, C., Tadich, A., Yin, Y., Zheng, C., Hellerstedt, J., Grubisic-Cabo, A., Tang, S., Mo, S.-K., Riley, J., Huwald, E., Medhekar, N.V., Fuhrer, M.S., Edmonds, M.T., Electronic band structure of in-plane ferroelectric van der Waals $\beta^{'}$In2Se3, ACS Applied Electronic Materials, 2020, 2, 213-219.
22. Kumar, D., Krull, C., Yin, Y., Medhekar, N.V., Schiffrin, A., Electric field control of molecular charge state in a single-component 2D organic nanoarray, ACS Nano, 2019, 13, 11882-11890.
23. Yin, Y., Fuhrer, M.S., Medhekar, N.V., Selective control of surface spin current in topological pyrite-type OsX_2 (X= Se, Te) crystals, npj Quantum Materials, 2019, 4, 47.
24. Haque, F., Zavabeti, A., Zhang, B.Y., Datta, R.S., Yin, Y., Yi, Z., Wang, Y., Mahmood, N., Pillai, N., Syed, N., Khan, H., Jannat, A., Wang, N., Medhekar, N., Kalantar-Zadeh, K., Ou, J.Z., Ordered intracrystalline pores in planar molybdenum oxide for enhanced alkaline hydrogen evolution, Journal of Materials Chemistry A, 2019, 7, 257-268.
25. Schiffrin, A., Capsoni, M., Farahi, G., Wang, C., Krull, C., Castelli, M., Roussy, T., Cochrane, K.A., Yin, Y., Medhekar, N.V., Fuhrer, N., Shaw, A.Q., Ji, W., Burke, S.A., Designing Optoelectronic Properties by On-Surface Synthesis: Formation and Electronic Structure of an Iron–Terpyridine Macromolecular Complex, ACS Nano, 2018, 12, 6545-6553.
26. Deng, J., Yin, Y., Niu, H., Ding, X., Sun, J., Medhekar, N.V., The edge stresses and phase transitions for magnetic BN zigzag nanoribbons, Scientific Reports, 2017, 7, 7855.
27. Yin, Y., Cervenka, J., Medhekar, N.V., Molecular dipole-driven electronic structure modifications of DNA/RNA nucleobases on graphene, The Journal of Physical Chemistry Letters, 2017, 8, 3087-3094.
28. Mukherjee, S., Manna, B., Desai, A.V., Yin, Y., Krishna, R., Babarao, R., Ghosh, S.K., Harnessing Lewis acidic open metal sites of metal–organic frameworks: the foremost route to achieve highly selective benzene sorption over cyclohexane, Chemical Communications, 2016, 52, 8215-8218.
29. Van Embden, J., Bourgeois, L., Della Gaspera, E., Waddington, L., Yin, Y., Medhekar, N.V., Jasieniak, J.J., Chesman, A.S., The formation mechanism of Janus nanostructures in one-pot reactions: the case of Ag–Ag_8GeS_6, Journal of Materials Chemistry A, 2016, 4, 7060-7070.
30. Yin, Y., Cervenka, J., Medhekar, N.V., Tunable hybridization between electronic states of graphene and physisorbed hexacene, The Journal of Physical Chemistry C, 2015, 119, 19526-19534.
31. Cervenka, J., Budi, A., Dontschuk, N., Stacey, A., Tadich, A., Rietwyk, K.J., Schenk, A., Edmonds, M.T., Yin, Y., Medhekar, N., Kalbac, M., Pakes, C.I.,Graphene field effect transistor as a probe of electronic structure and charge transfer at organic molecule–graphene interfaces, Nanoscale, 2015, 7, 1471-1478.

Skills

■□□□□ basic knowledge
■■□□□ intermediate knowledge with some project experience
■■■□□ extensive project experience
■■■■□ deepened expert knowledge
■■■■■ expert / specialist

	Level	Skill	Years	Comment
Programming Language:	■■■■□	Python	7	*Experienced user in scientific computing and data analysis with Python.*

	■■■□□	Fortran	7	*Strong background in writing and modifying large Fortran projects for scientific computing (e.g., WannierTools).*
	■■□□□	MATLAB	10+	*Good knowledge of using MATLAB for numerical modeling and data analysis.*
	■□□□□	C/C++	10+	*Basic understanding of C/C++ and capable of writing and modifying small programs.*
	■■■■□	LaTeX	10+	*Proficient in using LaTeX for writing papers and creating professional documents, including this CV.*
OS:	■■■■□	Linux	10+	*Experienced user in supercomputing systems and running parallel calculations.*
Simulation Package:	■■■■■	VASP	10+	*Expert in first principles calculations.*
	■■■■■	wannier90	7	*Expert in Wannierization and analysis based on Wannier-TB models*
	■■□□□	Materials Studio	3	*Basic knowledge in making atomic models and running calculations.*
	■■□□□	LAMMPS	2	*Basic knowledge of performing molecular dynamics calculations.*

Prizes, Honours and Awards

2018 FLEET Annual Workshop Best Poster Award

2012 I. J. Polmear Materials Engineering Prize

2012 Institute of Materials Engineering Australasia (IMEA) Award

Invited Keynote and Speaker Addresses

2021 American Physical Society (APS) March Meeting: Tuning the Surface Spin Textures of Topological Materials

2021 American Physical Society (APS) March Meeting: Tight-binding Models for Two-dimensional Allotropes of Bismuth based on Wannier Functions

2018 4th International Conference on Two-Dimensional Materials (ICON-2DMAT 2018): Enhancing electronic fingerprints of physisorbed molecules of graphene

2017 FLEET Inaugural Annual Workshop: Exploring and Predicting New Topological Electronic Materials Based on First Principles Calculations

2014 Molecular Modelling 2014: Tunable Hybridisation Between the Electronic States of Graphene and Physisorbed Molecules

Grants and Other Professional Activities

2020 FLEET - MacDiarmid Collaborative Grant, sponsored by FLEET (Australia) and MacDiarmid Institute (New Zealand)

2023-2024 NCI Computational Scheme: Exploring new approaches of modeling defects in materials, 550K CPU hours

Languages

Chinese Native or bilingual proficiency

English Professional working proficiency