Yuefeng Yin 尹越峰

Research Fellow (Quantum Physics + Computational Materials Science)

Department of Materials Science and Engineering, Monash University, Australia

I **use and develop the latest advanced computational methods** to address challenging topics in condensed matter physics and materials science. I strive to enhance the computing power of the future by discovering novel material candidates that exhibit ultralow energy consumption while delivering lightning-fast transport.

I believe in the power of integrating knowledge from different fields to achieve a common good. The future of research should be envisioned as a collective of researchers, each shining their talent through their unique skills, forming an interdisciplinary effort. I am also committed to spreading and sharing knowledge with the general public, particularly by translating complex research concepts into plain language

I have extensive experience in collaboration with fellow theorists, experimental researchers and industrial partners. So far I have published 31 peer-reviewed original research articles in the fields of Quantum Physics, Computational Materials Science, and Physical Chemistry.

yyfforce@gmail.com
yuefeng.yin@monash.edu
CV PDF
@rdortk
@yyfforce
Yuefeng Yin
Google Scholar

RESEARCH PROJECTS

May 2017 — Current

Developing DFT-Tight Binding Workflows for Quantum Physics

Codes/Packages Applied: *Python, Fortran, VASP, wannier90, MATLAB, C*

In this project, **I used advanced modeling techniques, including DFT and tight-binding methods, to develop a simple and universal 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.

Selected Research Outputs:

Extracting novel spin transport pattern from topological crystalline insulators: PDF
Effective tight-binding models for two-dimensional bismuth: PDF
Proposing a new type of topological transistor enabling fast switch: PDF

May 2017 — Current

Discovering New Topological Materials For Spintronics

Codes/Packages Applied: *VASP, wannier90, Python, Fortran, MATLAB*

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.

Selected Research Outputs:

Theoretical prediction of a new pyrite-type crystal with novel surface spin texture: PDF
Magnetic alloy for room temperature spintronics: PDF
Thickness-dependent electronic response in magnetic vdW thin layers: PDF

Mar. 2012— 2018

Change Graphene For Better Electronics
Codes/Packages Applied: *VASP, Python, MATLAB*

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.

Selected Research Outputs:
Graphene for next-generagtion DNA/RNA sensing and sequencing: PDF
Making Graphene-based heterostructures for next-generation electrodes: PDF

Mar. 2012— Current

2D Materials Beyond Graphene
Codes/Packages Applied: *VASP, wannier90*

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.

Selected Research Outputs:
Optoelectronics growing from 2D transition metal dichalcogenide: PDF
Assembly of 2D Kagome crystals: PDF

EDUCATION

Mar. 2012 — May 2016

Ph.D. in Materials Science and Engineering
Monash University, Melbourne, Victoria, Australia
Thesis: *Tailoring the electronic structure of graphene via molecular adsorption*
Advisor: Nikhil Medhekar, Co-advisor: Jiri Cervenka
[Thesis Project Page] [Thesis]

Sep. 2007 — Dec. 2011

B.Eng. in Materials Science and Enginnering (2+2 Program)
Monash University / Central South University, Melbourne, Victoria, Australia / Changsha, Hunan, China
Thesis: *Molecular Dynamics Simulation of Graphene and Related Materials*
[Thesis]

RESEARCH EXPERIENCE

Oct 2024 — Current

Monash University, Melbourne, Victoria, Australia
Senior Research Fellow, Department of Materials Science and Engineering / School of Physics and Astronomy
Conducting research in 2D materials and computational methodology development.

May 2017 — Aug 2024 Current

Monash University, Melbourne, Victoria, Australia
Research Fellow, Department of Materials Science and Engineering / School of Physics and

Research Fellow, Department of Materials Science and Engineering / School of Physics and Astronomy

Mentor: Nikhil V. Medhekar, Michael S. Fuhrer

Conducting research in topological materials under ARC Centre of Excellence in Future Low-Energy Electronic Technologies (FLEET).

Nov. 2010 — Mar. 2011

Commonwealth Scientific and Industrial Research Organisation (CSIRO), Melbourne, Victoria, Australia

Research Associate, CSIRO Mineral Processing

Mentor: Shouyi Sun

Measuring thermal properties of molten salt mixtures used in concentrated solar power

PUBLICATIONS

Publication Summary

I have published 36 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 887 citations with an h-index of 15.

5 Representative Publications

5

Extracting Unconventional Spin Texture in Two Dimensional Topological Crystalline Insulator Bismuthene via Tuning Bulk-Edge Interactions

Yuefeng Yin, Chutian Wang, Michael S. Fuhrer, Nikhil V. Medhekar

Materials Today Physics, *2023, 36, 101168.*

[Web] [PDF]

First systematic study of how bulk-edge interactions affects edge tranport in 2D topological materials and reveals coexistence of unconventional and coventional helical states in topological crystalline insulators.

4

Gigantic Anisotropy of Self-Induced Spin-Orbit Torque in Weyl Ferromagnet Co_2MnGa

Motomi Aoki, Yuefeng Yin, Simon Granville, Yao Zhang, Nikhil V. Medhekar, Livio Leiva, Ryo Ohshima, Yuichiro Ando, Masashi Shiraishi

Nano Letters, *2023, 15, 6951.*

[Web] [PDF]

Excellent agreement between theory and experiment in predicting the anisotropy of spin-orbit torque in Weyl ferromagnet Co_2MnGa.

3

Localized Wannier Function Based Tight-Binding Models for Two-Dimensional Allotropes of Bismuth

Qile Li, Jackson S. Smith, Yuefeng Yin, Chutian Wang, Mykhailo V. Klymenko, Jared H. Cole, Nikhil V. Medhekar

New Journal of Physics, *2021, 6, 26371.*

[Web] [PDF]

Developing a workfow of transforming first-principles calculations into simplified and symmetrized tight-binding models for two-dimensional allotropes of bismuth.

2

Selective Control of Surface Spin Current in Topological Pyrite-Type OsX_2 (X = Se, Te) Crystals

Yuefeng Yin, Michael S. Fuhrer, Nikhil V. Medhekar

npj Quantum Materials, *2019, 4, 47.*

[Web] [PDF] [Code]

[Web] [PDF] [Code]

First theoretical prediction of anisotropic surface spin states in a pristine non-magnetic material.

1

Molecular Dipole-Driven Electronic Structure Modifications of DNA/RNA Nucleobases on Graphene

Yuefeng Yin, Jiri Cervenka, Nikhil V. Medhekar

Journal of Physical Chemistry Letters, *2017, 8, 3087.*

[Web] [PDF]

Summarizing highlights of my Ph.D. work on the electronic structure modifications of graphene via molecular adsorption.

Full Publication List

42

Uncovering complex phonon interactions in $Mg_3Bi_{2-x}Sb_x$: topology and avoided crossings

Lei Chen, Yuefeng Yin, Ting Lu, Huangshui Ma, Shuxian Zhang, Xinyue Zhang, Zhiwei Chen, Siqi Lin, Siqi Huo, Shengqing Xia, Richard A. Mole, Dehong Yu, Kirrily C. Rule, Weiyao Zhao, Julie Karel, Pingan Song, John Bell, Min Hong

Nature Communications, *2026, , .*

[Project] [中文页面] [Web] [PDF]

41

Efficient and Robust p-Type Transistor Based on Ultrawide-Bandgap Semiconductor

Kaijian Xing, Zherui Yang, Weiyao Zhao, Yuefeng Yin, Huiping Han, Shanhu Wang, Shifan Wang, James Bullock, Alastair Stacey, James A. Belcourt, Sergey Rubanov, Hang Yin, David A. Broadway, Jean-Philippe Tetienne, Xinmao Yin, Liang Wu, Dong-Chen Qi, Michael S. Fuhrer, Qingdong Ou, Xiao Renshaw Wang

ACS Nano, *2026, 20, 7343-7354.*

[Web] [PDF]

40

Band Structure Engineering to Optimize Spin-Wave Propagation in Weyl ferromagnet $Co_2MnGa_{1-x}Ge_x$

Jinlong Wang, Yao Zhang, Junfeng Hu, He Song, Xiaozhen Sun, Xiangrui Meng, Ziyue Xu, Yuefeng Yin, Tianyu Yang, Lutong Sheng, Jilei Chen, Song Liu, Peng Li, Peng Gao, Nikhil V. Medhekar, Dapeng Yu, Simon Granville, Haiming Yu

Advanced Materials, *2025, 37, 2505704.*

[Web] [PDF]

39

Edge state stabilization and control in 2D topological crystalline insulators

Chutian Wang, Yuefeng Yin, Thanh Tung Huynh, Michael S. Fuhrer, Nikhil V. Medhekar

Materials Today Physics, *2025, 59, 101897.*

[Web] [PDF]

38

Giant temperature-independent ultraviolet circular dichroism in Co_2MnX (X = Ga, Ge) Heusler magnetic thin films

Yao Zhang, Jie Sung, Yuefeng Yin, Yu-Ying Chang, Nikhil V. Medhekar, Simon Granville, Hua-Shu Hsu

Physical Review Applied, *2025, 24, 14378.*

[Web] [PDF]

37

Room temperature quantum metric effect in $TbMn_6Sn_6$

Weiyao Zhao, Kaijian Xing, Yufei Zhao, Lei Chen, Min Hong, Yuefeng Yin, Yang Liu, Dang Khoa Le, Jacob Gayles, Fang Tang, Yong Fang, Binghai Yan, Julie Karel

Nature Communications, *2025, 16, 6837.*

[Web] [PDF]

36

Giant berry curvature in amorphous ferromagnet Co_2MnGa

Weiyao Zhao, Yao Zhang, Yuefeng Yin, Kaijian Xing, Shengqiang Zhou, Abdulhakim Bake, Golrokh Akhgar, David Cortie, Lei Chen, Xiaolin Wang, Kirrily C. Rule, Nikhil V. Medhekar, Simon Granville, Julie Karel
Matter, *2025, 8, 101988*.

[Web] [PDF]

35

Pick-and-Place Transfer of Arbitrary-Metal Electrodes for van der Waals Device Fabrication

Kaijian Xing, Daniel McEwen, Yuefeng Yin, Weiyao Zhao, Abdulhakim Bake, David Cortie, Jingying Liu, Thi-Hai-Yen Vu, Yi-Hsun Chen, James Hone, Alastair Stacey, Mark T. Edmonds, Nikhil V. Medhekar, Kenji Watanabe, Takashi Taniguchi, Qingdong Ou, Dong-Chen Qi, Michael S. Fuhrer
ACS Nano, *2025, 19, 3579*.

[Web] [PDF]

34

Generic Approach to Intrinsic Magnetic Second-Order Topological Insulators via Inverted p–d Orbitals

Zhao Liu, Bing Liu, Yuefeng Yin, Nikhil V. Medhekar
Nano Letters, *2024, 24, 11295*.

[Web] [PDF]

33

Electrically Controlled High Sensitivity Strain Modulation in MoS_2 Field-Effect Transistors via a Piezoelectric Thin Film on Silicon Substrates

Abin Varghese, Adityanarayan H. Pandey, Pooja Sharma, Yuefeng Yin, Nikhil V. Medhekar, Saurabh Lodha
Nano Letters, *2024, 24, 8472*.

[Web] [PDF]

32

Electron–phonon interactions at the topological edge states in single bilayer Bi (111)

Enamul Haque, Yuefeng Yin, Nikhil V. Medhekar
Nanoscale, *2024, 16, 17442*.

[Web] [PDF]

31

Origin of Different Piezoelectric Responses in Elemental Sb and Bi Monolayers

Yunfei Hong, Junkai Deng, Qi Kong, Yuefeng Yin, Xiangdong Ding, Jun Sun, Jefferson Zhe Liu
Physical Review B, *2024, 109, 14980*.

[Web] [PDF]

30

Quasi-free-standing AA-stacked Bilayer Graphene Induced by Calcium Intercalation of the Graphene-Silicon Carbide Interface

Antonija Grubisic-Cabo, Jimmy C. Kotsakidis, Yuefeng Yin, Anton Tadich, Matthew Haldon, Sean Solari, John Riley, Eric Huwald, Kevin M. Daniels, Rachael L. Myers-Ward, Mark T. Edmonds, Nikhil V. Medhekar, D. Kurt Gaskill, Michael S. Fuhrer
Frontiers in Nanotechnology, *2024, 5, 1333127*.

[Web] [PDF]

29

Using Optical Spectroscopy to Probe the Impact of Atomic Disorder on the Heusler Alloy Co_2MnGa

Ben Mallett, Yao Zhang, Catherine Pot, Kiri Van Koughnet, Blake Stanley, Robert G. Buckley, Annette Koo, Yuefeng Yin, Nikhil V. Medhekar, Simon Granville
Physical Review Materials, *2023, 7, 094203*.

[Web] [PDF]

28

Extracting Unconventional Spin Texture in Two Dimensional Topological Crystalline Insulator Bismuthene via Tuning Bulk-Edge Interactions

Yuefeng Yin, Chutian Wang, Michael S. Fuhrer, Nikhil V. Medhekar

Materials Today Physics, *2023, 36, 101168*.

[Web] [PDF]

27

Gigantic Anisotropy of Self-Induced Spin-Orbit Torque in Weyl Ferromagnet Co_2MnGa

Motomi Aoki, Yuefeng Yin, Simon Granville, Yao Zhang, Nikhil V. Medhekar, Livio Leiva, Ryo Ohshima, Yuichiro Ando, Masashi Shiraishi

Nano Letters, *2023, 15, 6951*.

[Web] [PDF]

26

Giant Piezoresistivity in a van der Waals Material Induced by Intralayer Atomic Motions

Lingyun Tang, Zhongquan Mao, Chutian Wang, Qi Fu, Chen Wang, Yichi Zhang, Jingyi Shen, Yuefeng Yin, Bin Shen, Dayong Tan, Qian Li, Yonggang Wang, Nikhil V. Medhekar, Jie Wu, Huiqiu Yuan, Yanchun Li, Michael S. Fuhrer, Changxi Zheng

Nature Communications, *2023, 14, 1519*.

[Web] [PDF]

25

Wavelength-Controlled Photocurrent Polarity Switching in BP-MoS_2 Heterostructure

Himani Jawa, Abin Varghese, Sayantan Ghosh, Srilagna Sahoo, Yuefeng Yin, Nikhil V. Medhekar, Saurabh Lodha

Advanced Functional Materials, *2022, 32, 2112696*.

[Web] [PDF]

24

Near-Infrared and Visible-Range Optoelectronics in 2D Hybrid Perovskite/Transition Metal Dichalcogenide Heterostructures

Abin Varghese, Yuefeng Yin, Mingchao Wang, Saurabh Lodha, Nikhil V. Medhekar

Advanced Materials Interfaces, *2022, 9, 2102174*.

[Web] [PDF]

23

Polarity-Tunable Photocurrent through Band Alignment Engineering in a High-Speed $WSe_2/SnSe_2$ Diode with Large Negative Responsivity

Sayantan Ghosh, Abin Varghese, Himani Jawa, Yuefeng Yin, Nikhil V. Medhekar, Saurabh Lodha

ACS Nano, *2022, 16, 4578*.

[Web] [PDF]

22

Proposal for a Negative Capacitance Topological Quantum Field-Effect Transistor

Michael S. Fuhrer, Mark T. Edmonds, Dimitrie Culcer, Muhammad Nadeem, Xiaolin Wang, Nikhil V. Medhekar, Yuefeng Yin, Jared H. Cole

2021 IEEE International Electron Devices Meeting (IEDM), *2021, 38, 2.1*.

[Web] [PDF]

21

Manifestation of Strongly Correlated Electrons in a 2D Kagome Metal–Organic Framework

Dhaneesh Kumar, Jack Hellerstedt, Bernard Field, Benjamin Lowe, Yuefeng Yin, Nikhil V. Medhekar, Agustin Schiffrin

Advanced Functional Materials, *2021, 31, 2106474*.

[Web] [PDF]

20

Crossover from 2D Ferromagnetic Insulator to Wide Band Gap Quantum Anomalous Hall Insulator in Ultrathin $MnBi_2Te_4$

Chi Xuan Trang, Qile Li, Yuefeng Yin, Jinwoong Hwang, Golrokh Akhgar, Iolanda Di Bernardo, Antonija Grubišić-Čabo, Anton Tadich, Michael S. Fuhrer, Sung-Kwan Mo, Nikhil V. Medhekar, Mark T. Edmonds
ACS Nano, *2021, 15, 13444*.

[Web] [PDF]

19

Localized Wannier Function Based Tight-Binding Models for Two-Dimensional Allotropes of Bismuth

Qile Li, Jackson S. Smith, Yuefeng Yin, Chutian Wang, Mykhailo V. Klymenko, Jared H. Cole, Nikhil V. Medhekar
New Journal of Physics, *2021, 6, 26371*.

[Web] [PDF]

18

Magnesium-Intercalated Graphene on SiC: Highly n-doped Air-Stable Bilayer Graphene at Extreme Displacement Fields

Antonija Grubišić-Čabo, Jimmy C. Kotsakidis, Yuefeng Yin, Anton Tadich, Matthew Haldon, Sean Solari, Iolanda Di Bernardo, Kevin M. Daniels, John Riley, Eric Huwald, Mark T. Edmonds, Rachael Myers-Ward, Nikhil V. Medhekar, D Kurt Gaskill, Michael S. Fuhrer
Applied Surface Science, *2021, 541, 148612*.

[Web] [PDF]

17

Probing the Dynamic Structural Changes of DNA Using Ultrafast Laser Pulse in Graphene-Based Optofluidic Device

Bannur N. Shivananju, Lu Zhou, Yuefeng Yin, Wenzhi Yu, Babar Shabbir, Haoran Mu, Xiaozhi Bao, Yiqiu Zhang, Sun Tian, Qingdong Ou, Shaojuan Li, Mohammad M. Hossain, Yupeng Zhang, Huaiyu Shao, Guichuan Xing, Nikhil V. Medhekar, Chang-Ming Li, Jian Liu, Qiaoliang Bao
InfoMat, *2021, 3, 316*.

[Web] [PDF]

16

Berry Curvature Origin of the Thickness-Dependent Anomalous Hall Effect in a Ferromagnetic Weyl Semimetal

Yao Zhang, Yuefeng Yin, Guy Dubuis, Tane Butler, Nikhil V. Medhekar, Simon Granville
npj Quantum Materials, *2021, 6, 17*.

[Web] [PDF]

15

First-Principles Study of Mechanical and Optical Properties for ZnS1– xOx Alloying Compounds

Junfu Qi, Yuefeng Yin, Xiangdong Ding, Jun Sun, Junkai Deng
Materials Today Communications, *2020, 24, 101259*.

[Web] [PDF]

14

Intrinsic-Strain-Induced Curling of Free-Standing Two-Dimensional Janus MoSSe Quantum Dots

Han Ye, Yunzhen Zhang, Anran Wei, Delong Han, Yumin Liu, Wenjun Liu, Yuefeng Yin, Mingchao Wang
Applied Surface Science, *2020, 519, 146251*.

[Web] [PDF]

13

Freestanding n-Doped Graphene via Intercalation of Calcium and Magnesium into the Buffer Layer–SiC(0001) Interface

Jimmy C. Kotsakidis, Antonija Grubišić-Čabo, Yuefeng Yin, Anton Tadich, Rachael L. Myers-Ward, Matthew DeJarld, Shojan P. Pavunny, Marc Currie, Kevin M. Daniels, Chang Liu, Mark T. Edmonds, Nikhil V. Medhekar, D Kurt Gaskill, Amadeo L. Vázquez de Parga, Michael S. Fuhrer
Chemistry of Materials, *2020, 32, 6464*.

[Web] [PDF]

12

Chemical Switching of Low-Loss Phonon Polaritons in α-MoO3 by Hydrogen Intercalation

Yingjie Wu, Qingdong Ou, Yuefeng Yin, Yun Li, Weiliang Ma, Wenzhi Yu, Guanyu Liu, Xiaoqiang Cui, Xiaozhi Bao, Jiahua Duan, Gonzalo Álvarez-Pérez, Zhigao Dai, Babar Shabbir, Nikhil Medhekar, Xiangping Li, Chang-Ming Li, Pablo Alonso-González, Qiaoliang Bao

Nature Communications, *2020, 11, 2646*.

[Web] [PDF]

11

Electronic Band Structure of In-Plane Ferroelectric van der Waals β′-In2Se3

James L. Collins, Chutian Wang, Anton Tadich, Yuefeng Yin, Changxi Zheng, Jack Hellerstedt, Antonija Grubisic-Cabo, Shujie Tang, Sung-Kwan Mo, John Riley, Eric Huwald, Nikhil V. Medhekar, Michael S. Fuhrer, Mark T. Edmonds

ACS Applied Electronic Materials, *2020, 2, 213*.

[Web] [PDF]

10

Selective Control of Surface Spin Current in Topological Pyrite-Type OsX_2 (X = Se, Te) Crystals

Yuefeng Yin, Michael S. Fuhrer, Nikhil V. Medhekar

npj Quantum Materials, *2019, 4, 47*.

[Web] [PDF] [Code]

9

Designing Optoelectronic Properties by On-Surface Synthesis: Formation and Electronic Structure of an Iron–Terpyridine Macromolecular Complex

Dhaneesh Kumar, Cornelius Krull, Yuefeng Yin, Nikhil V. Medhekar, Agustin Schiffrin

ACS Nano, *2019, 13, 11882*.

[Web] [PDF]

8

Designing Optoelectronic Properties by On-Surface Synthesis: Formation and Electronic Structure of an Iron–Terpyridine Macromolecular Complex

Farjana Haque, Ali Zavabeti, Bao Yue Zhang, Robi S. Datta, Yuefeng Yin, Zhifeng Yi, Yichao Wang, Nasir Mahmood, Naresh Pillai, Nitu Syed, Hareem Khan, Azmira Jannat, Ning Wang, Nikhil V. Medhekar, Kourosh Kalantar-zadeh, Jian Zhen Ou

Journal of Materials Chemistry A, *2019, 7, 257*.

[Web] [PDF]

7

Designing Optoelectronic Properties by On-Surface Synthesis: Formation and Electronic Structure of an Iron–Terpyridine Macromolecular Complex

Agustin Schiffrin, Martina Capsoni, Gelareh Farahi, Chen-Guang Wang, Cornelius Krull, Marina Castelli, Tanya Roussy, Katherine A. Cochrane, Yuefeng Yin, Nikhil V. Medhekar, Michael Fuhrer, Adam Q. Shaw, Wei Ji, Sarah A. Burke

ACS Nano, *2018, 12, 6545*.

[Web] [PDF]

6

The Edge Stresses and Phase Transitions for Magnetic BN Zigzag Nanoribbons

Junkai Deng, Yuefeng Yin, Huanhuan Niu, Xiangdong Ding, Jun Sun, Nikhil V. Medhekar

Scientific Reports, *2017, 7, 7855*.

[Web] [PDF]

5

Molecular Dipole-Driven Electronic Structure Modifications of DNA/RNA Nucleobases on Graphene

Yuefeng Yin, Jiri Cervenka, Nikhil V. Medhekar

Journal of Physical Chemistry Letters, *2017, 8, 3087*.

[Web] [PDF]

4

Harnessing Lewis Acidic Open Metal Sites of Metal–Organic Frameworks: the Foremost Route to Achieve Highly Selective Benzene Sorption Over Cyclohexane

Soumya Mukherjee, Biplab Manna, Aamod V. Desai, Yuefeng Yin, Rajamani Krishna, Ravichandar Babarao, Sujit K. Ghosh

Chemical Communications, *2016, 52, 8215*.

[Web] [PDF]

3

The Formation Mechanism of Janus Nanostructures in One-Pot Reactions: the Case of Ag–Ag_8GeS_6

Joel Van Embden, Laure Bourgeois, Enrico Della Gaspera, Lynne Waddington, Yuefeng Yin, Nikhil V. Medhekar, Jacek J. Jasieniak, Anthony SR. Chesman

Journal of Materials Chemistry A, *2016, 4, 7060*.

[Web] [PDF]

2

Tunable Hybridization Between Electronic States of Graphene and Physisorbed Hexacene

Yuefeng Yin, Jiri Cervenka, Nikhil V. Medhekar

Journal of Physical Chemistry C, *2015, 119, 19526*.

[Web] [PDF]

1

Graphene Field Effect Transistor as a Probe of Electronic Structure and Charge Transfer at Organic Molecule–Graphene Interfaces

Jiri Cervenka, Akin Budi, Nikolai Dontschuk, Alastair Stacey, Anton Tadich, Kevin J. Rietwyk, Alex Schenk, Mark T. Edmonds, Yuefeng Yin, Nikhil V. Medhekar, Martin Kalbac, Chris I. Pakes

Nanoscale, *2015, 7, 1471*.

[Web] [PDF]

CONFERENCE

6

Tuning the Edge States of Bismuthene via Substrate Effects

Chutian Wang, Yuefeng Yin, Michael S. Fuhrer, Nikhil V. Medhekar

American Physical Society (APS) March Meeting. Virtual, Mar. 2021.

[Conference Page]

5

Tight-Binding Models for Two-Dimensional Allotropes of Bismuth-based on Localized Wannier Functions

Qile Li, Jackson Smith, Yuefeng Yin, Chutian Wang, Mykhailo Klymenko, Jared Cole, Nikhil V. Medhekar

American Physical Society (APS) March Meeting. Virtual, Mar. 2021.

[Conference Page]

4

Tuning the Surface Spin Textures of Topological Materials

Yuefeng Yin, Michael S. Fuhrer, Nikhil V. Medhekar

American Physical Society (APS) March Meeting. Virtual, Mar. 2021.

[Conference Page]

3

Enhancing Electronic Fingerprints of Physisorbed Molecules of Graphene

Yuefeng Yin

4th International Conference on Two-Dimensional Materials (ICON-2DMAT 2018). Melbourne, Victoria, Australia, Dec. 2018.

2

Exploring and Predicting New Topological Electronic Materials Based on First Principles Calculations

Yuefeng Yin

FLEET Inaugural Annual Workshop. Lorne, Victoria, Australia, Dec. 2017.

1

Tunable Hybridisation Between the Electronic States of Graphene and Physisorbed Molecules

Yuefeng Yin

Molecular Modelling 2014. Gold Coast, Queensland, Australia, Jul. 2014.

GRANTS AND FUNDINGS

2023 — Current

Exploring New Approaches of Modeling Defects in Materials

NCI Adapter Scheme/NCI-Monash Computational Scheme

Funded 3M+ SU CPU hours (approximately A$200,000 in research expense)

2025 — Current

Understanding the interfacial interactions for semiconductor-metal/semiconductor contact

Pawsey Fast Track Scheme

Funded 500K SU CPU hours (approximately A$30,000 in research expense)

2020-2023

Topological properties of Anisotropic Weyl semi-metal Co_2MnGa

FLEET-MacDiarmid Collaborative Grant

Co-PIs: Dr. Simon Granville, Victoria University of Wellington, New Zealand.

Funded A$10,750 to conduct short-term collaborative visits to Victoria University of Wellington, New Zealand.

TEACHING

2017 - Current

Lecturer

Monash University / Central South University, Melbourne, Victoria, Australia / Changsha, Hunan, China

Computational Materials Science, Materials Characterization, and Fundamentals of Materials Science

[🔗 Course Materials]

2012 - 2016

Graduate Teaching Assistant

Monash University, Melbourne, Victoria, Australia

Modeling of Materials, and Materials Characterization

MENTORING

2025 - Current

Hanqi Wang

Ph.D. Candidate, Materials Science and Engineering, Monash University

Ph.D. co-supervisor

2025 - Current

Minh Tien Le

Ph.D. Candidate, Materials Science and Engineering, Monash University

Ph.D. co-supervisor

2025 - Current

Rahul Awale

Joint Ph.D. Candidate in Monash University and Indian Institute of Technology, Bombay

Joint Ph.D. candidate in Monash University and Indian Institute of Technology, Bombay
Ph.D. mentor

2024 - Current

Tung Huynh
Ph.D. Candidate, Materials Science and Engineering, Monash University
Ph.D. mentor

2021 - 2025

Ziyuan Zhao
Ph.D. in Materials Science and Engineering, Monash University
Ph.D. co-supervisor

2021 - 2025

Enamul Haque
Ph.D. in Materials Science and Engineering, Monash University
Ph.D. mentor (through FLEET projects)

2019 - 2023

Bernard Field
Ph.D. in Physics, Monash University
Ph.D. mentor (through FLEET projects)

2019 - 2023

Abin Varghese
Joint Ph.D. in Materials Science and Engineering, Monash University and Ph.D. in Electric Engineering, Indian Institute of Technology, Bombay
Ph.D. mentor (through FLEET projects)

2018 - 2022

Chutian Wang
Ph.D. in Materials Science and Engineering, Monash University
Ph.D. mentor (through FLEET projects)

2019

Qile Li
Ph.D. in Physics, Monash University
Undergraduate Final Year Project co-supervisor (with Prof. Nikhil V. Medhekar)

PRESS

Sep. 2023

"Topological Gardening To Achieve Unexpected Spin Transport," Materials Australia

Dec. 2019

"New spin directions in pyrite an encouraging sign for future spintronics," Australian Research Council (ARC) Newsletter

Nov. 2019

"The Hetero-Interface is the Device: A Computational Approach," FLEET website

REFERENCES

Dr. Nikhil V. Medhekar, Professor
Department of Materials Science and Engineering
Monash University, Melbourne, Victoria, Australia
Group Homepage

Dr. Michael S. Fuhrer, Professor, FAA
School of Physics and Astronomy
Monash University, Melbourne, Victoria, Australia
Monash Profile

Dr. Simon Granville, Senior Scientist

Dr. Simon Granville, Senior Scientist
Robinson Research Institute
Victoria University of Wellington, Wellington, New Zealand
VUW Profile