Nikhil Medhekar

Curriculum Vitae

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Education

2009	Ph.D. (Engineering), Brown University, USA.
2006	Sc.M. (Applied Mathematics), Brown University, USA.
2002	M.Tech. (Mechanical Engineering), Indian Institute of Technology Bombay, India.
2000	B.E. (Mechanical Engineering), University of Pune, India.

Current Appointments

2017–	Associate Professor, Dept. of Materials Science & Engineering, Monash University.

Past Appointments

2018–2020	Deputy Associate Dean of Education (Postgraduate Courses), Faculty of Engineering, Monash University.
2010–2016	Senior Lecturer, Department of Materials Science & Engineering, Monash University.
2009–2010	Postdoctoral Research Fellow, Brown University, USA.
2003–2008	Graduate Research Assistant, Brown University, USA.
2002–2003	Mechanical Engineer, General Electric Corporate Research, Bangalore, India.
2000–2002	Graduate Research Assistant, Indian Institute of Technology, Bombay, India.

Honours and Awards

2014	Young Tall Poppy Science Award, Australian Institute of Policy and Science.
2008	Graduate Silver Award for outstanding graduate research, Materials Research Society, USA.
2008	William N. Findley Award for best research paper, Brown University, USA.
2002	Ashok Chaturvedi and P. M. Natu Memorial Awards for Outstanding Performance, Indian Institute of Technology, Bombay, India.
2002	Edison Engineering Development Program at General Electric Corporate Research.
2000	Forbes Marshal Award for Best Undergraduate Thesis, University of Pune, India.

Research – Discovery and Design of Next Generation Materials

My research focuses on physics, chemistry and engineering of materials for next-generation applications in energy storage, optoelectronics and multifunctional devices. The question driving my group's research concentrates on how a material's structure and chemistry at the atomic level controls its performance in practical applications. To address this, we employ a wide variety of modelling and simulation methods ranging from quantum mechanical methods to large scale molecular dynamics and data-driven methods, using massively parallel computing facilities.

Research Leadership Summary

- My research expertise is unique at Monash. I independently founded the Computational Materials group at Monash and have established a vibrant, externally funded research program in materials discovery and design, a research area that is still developing in Australia. The research group has now grown to 10 PhD students, 2 postdoctoral researchers and a number of undergraduate researchers.
- I have established leadership in my field, having made notable contributions in modern understanding of the structure and properties of a diverse range of materials from semiconductors and two-dimensional materials, to metals and battery materials. The diversity in the application areas is a unique strength of my research program, and has enabled me to form a wide network of collaborations across science and engineering, both locally and internationally.

- I have successfully attracted an extensive portfolio of external research funding from the Australian Research Council (ARC), which include several Discovery Projects, large centres such as Centre of Excellence in Future Low Energy Technologies (ARC CoE FLEET) and Industrial Transformation Research Hub on Advanced Manufacturing of 2D Materials (ARC ITRH AM2D), as well as via highly competitive national grants for high performance computing resources which are critical for my research.
- My research leadership is well recognized internationally and locally, with several invitations for talks and keynote presentations, editorial responsibilities and organization of symposia and conferences. I have served on and chaired expert panels for selecting nationally competitive grants for resources on high performance computing facilities, a key research infrastructure for not just materials science and engineering, but also for fields such as astronomy and astrophysics, bioinformatics and climate modelling.

Grants and Research Support Summary

- >$40M in Australian Research Council's Funding, personal share >$4.5M.
- ~$175K in Monash University internal grants.
- ~$3.5M research support from the competitive National High Performance Computing Merit Allocation Grants (personal share).
- ~$120K in other research support.

A full list of research grants is available in the Appendix A1.

Research Output Summary

- 90 publications in top peer reviewed journals in materials science and engineering, including *Nature Nanotechnology*, *Advanced Materials*, *Nature Communications*, *Advanced Functional Materials*, *Nano Letters*, *ACS Nano*, *Journal of the American Chemical Society*, *Journal of Physical Chemistry Letters*, *Physical Review Letters*, *Journal of Materials Chemistry* and *Acta Materialia*. Nearly all of publications are in Q1 quality journals, and a number of them are in top 10% journals.
- 27 invited/keynote conference presentations and research talks.
- Total citations >4750, *h-index* 29 (Google Scholar), *m-index* 2.4 (*h-index* divided by years since PhD, Google Scholar). The citations are growing rapidly—in 2020 alone, my research received >780 citations. The average citation rate is ~53 (Google Scholar). The *Scival* 3-year (2018–2020) Field-Weighted Citation Index is 2.1.

A full list of publications is available in the Appendix A2, and a list of invited talks is provided in Appendix A3.

Research Supervision Summary

- I have closely supervised 12 PhD students to completion, who have all successfully commenced their careers in globally recognised academic institutions and industries.
- Several students and postdoctoral researchers that I have mentored have won prestigious awards, most notably the 2019 Monash University Vice Chancellor's Award for Thesis Excellence. As a dedicated research supervisor, I remain genuinely committed to be a lifelong mentor to my students, inspiring them towards success in their career as well as in their personal well-being.

A full list of current group members, group alumni and the awards won by them is available in the Appendix A4.

Education Leadership Summary

- I served as the Deputy Associate Dean of Education (GPG courses) in the Faculty of Engineering at Monash (mid 2018–Sep 2020). Key responsibilities and achievements include
    - Successfully led development and rollout of faculty-wide course Master of Professional Engineering. This course is Faculty's flagship masters course with external accreditation, and has seen a rapid growth in enrolment.
    - Served as a director, with a responsibility of the overall academic oversight, of masters courses in the Faculty of Engineering.

Major Service to Research Community

- Guest Associate Editor, Frontiers in Materials (2022–).

- Member, Organising Committee, Global Summit and Expo on Graphene and 2D Materials, Edinburgh, UK (Aug 2022).
- Member, Australia's National Computing Merit Allocation Scheme (2020-).
- Chair, Pawsey High Performance (Perth) Computing facility merit allocation committee (2017-2020).
- Member, Pawsey High Performance Computing facility Capital Refresh user group (2019-).
- Member, National Steering Committee on Integrated Computational Materials Engineering (2019).
- Organiser, Symposium on Advanced Materials for Carbon Capture and Gas Separations, Materials Research Society Spring meeting, Phoenix, USA (April 2018).
- Expert assessor for Australian Research Council's proposals (Discovery, Linkage Projects, DECRA and Future Fellowships), Austrian Research Fund, and Czech Republic Academy of Sciences.
- Expert reviewer for several peer-reviewed journals in materials science and engineering: ACS Nano, ACS Applied Materials and Interfaces, Journal of Power Sources, Journal of Physical Chemistry, ACTA Materialia, Nanoscale, Applied Physics Letters, Journal of Applied Physics, Physical Chemistry Chemical Physics, RSC Advances.
- External expert assessor for masters and PhD theses (UNSW, UQ, QUT, RMIT).
- External expert assessor for academic promotion applications (UNSW).

Teaching

- Modelling of Materials, year 4 (2014, 2016, 2020).
- Materials Characterisation and Modelling, year 3 (2011–2017).
- Mechanical Properties of Materials, year 2 (2021–).
- Structure Property Relationships in Materials, year 2 (2011–2014).
- Materials Engineering Final Year Projects, year 4 (2011–2021).
- Master of Advanced Engineering Research Projects (2016).

Outreach to Wider Community

- Outreach activities promoting study and careers in science and technology among the wider community and society. This was achieved via various platforms provided by the Tall Poppy Campaign, Australian Institute of Policy and Science, Melbourne Knowledge Week and University and Departmental outreach activities.
- I regularly participate and organise visits from secondary school students, immersion day, Open days etc.
- In formal roles, I have chaired the departmental Outreach committee (2014–2016), and the Outreach and Communications committee for ARC Centre of Excellence FLEET (2020–).

APPENDIX A1. Grants and Research Support

Australian Research Council (ARC) grants

2021–2025	M. Majumder and 8 Chief Investigators including N. V. Medhekar. "Advanced Manufacturing of 2D Materials (AM2D)" Industrial Transformation Research Hub IH210100025.	$4.4M
2017–2023	M. Fuhrer, and 17 Chief Investigators including N. V. Medhekar. "Future Low Energy Electronics Technologies." Centre of Excellence CE170100039.	$34.6M
2021–2023	L. Bourgeois, N. V. Medhekar and M. Weyland, "From One Structure to Another for Improved Materials Design." Discovery Project DP 210101451.	$476K
2016–2019	N. V. Medhekar, N. Birbilis and G. Williams. "Next Generation Batteries: Exploiting Divalent Magnesium." Discovery Project DP160103661.	$391K
2015–2017	L. Bourgeois and N. V. Medhekar. "Complex Interfaces and Solid-State Precipitation in Advanced Materials." Discovery Project DP150100558.	$374K
2013–2015	G. Simon, D. Li and N. V. Medhekar. "New Stimuli-Responsive Polymer Membranes using Graphene as a Multifunctional Scaffold." Discovery Project DP130102512.	$395K

Monash University Internal grants

2018	K. Pas and N. V. Medhekar. "New Haber-Bosch Processes for Ammonia Production using Sustainable Electrolytes." 2018 Faculty of Engineering and Faculty of Science Interdisciplinary Research Seed Fund Scheme.	$26K
2018	J. Karel, R. Engel-Herbert, N. V. Medhekar, V. Gopalan, N. Alem, "Design of Novel Materials and Material Heterostructures for Emerging Low Power Electronic and Magnetic Devices." Monash University–Penn State University 2018 Collaboration Development Fund.	$20K
2016	N. V. Medhekar. "Discovering Non-Toxic Hybrid Perovskite Materials for High-Efficiency Solar Cells." Monash University Faculty of Engineering Seed Grant.	$20K
2014	N. V. Medhekar. "Porous Aromatic Frameworks for High Performance Energy Storage." Monash University Faculty of Engineering Seed Grant.	$30K
2013	N. V. Medhekar. "Next Generation Battery Materials." Monash University Faculty of Engineering Seed Grant.	$30K
2012	N. V. Medhekar. "High Performance Graphene Based Polymer Nanocomposites." Monash University Faculty of Engineering Seed Grant.	$30K
2011	N. V. Medhekar. "Understanding Mechanisms of Graphene Growth." Monash University Faculty of Engineering Seed Grant.	$10K
2011	N. V. Medhekar. Monash University Faculty of Engineering New Staff Member Grant.	$8K

Nationally Competitive Computing grants (in kind)

2021	N. V. Medhekar. "In Silico Design of Nanoscale Energy Materials." Pawsey Energy and Resources Merit Allocation Grant.	$420k
2021	N. V. Medhekar. "Enabling Functional Properties of Nanomaterials using Atomistic Simulations." National Computing Merit Allocation Grant.	$220k
2020	N. V. Medhekar. "In Silico Design of Nanoscale Energy Materials." Pawsey Energy and Resources Merit Allocation Grant.	$350k
2020	N. V. Medhekar. "Enabling Functional Properties of Nanomaterials using Atomistic Simulations." National Computing Merit Allocation Grant.	$220k
2019	N. V. Medhekar. "In Silico Design of Nanoscale Energy Materials." Pawsey Energy and Resources Merit Allocation Grant.	$350k
2019	N. V. Medhekar. "Enabling Functional Properties of Nanomaterials using Atomistic Simulations." National Computing Merit Allocation Grant.	$150k
2018	N. V. Medhekar. "In Silico Design of Nanoscale Energy Materials." Pawsey Energy and Resources Merit Allocation Grant.	$200k
2018	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$350k
2017	N. V. Medhekar. "In Silico Design of Nanoscale Energy Materials." Pawsey Energy and Resources Merit Allocation Grant.	$160k
2017	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$200k

2016	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$150k
2015	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$100k
2014	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$120k
2013	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$120k
2012	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$20k
2011	N. V. Medhekar. "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	$10k

Allocation of 1 Service Unit (1 cpu-hr) is monetarily equivalent to $0.1.

Other research support

2013–2017	CSIRO support for PhD project at IITB-Monash Research Academy.	$75K
2013–2017	CSIRO support for PhD top up scholarship.	$40K

APPENDIX A2. Publications

Refereed Journal Papers

2021 [9 papers*]

90. Q. Li, J. Smith, Y. Yin, C.Wang, M. Klymenko, J. Cole and N. V. Medhekar, Localized Wannier function based tight-binding models for two-dimensional allotropes of bismuth, NEW JOURNAL OF PHYSICS 23, 063042 (2021).
89. D. Kumar, J. Hellerstedt, B. Field, B. Lowe, Y. Yin, N. V. Medhekar and A. Schiffrin, Manifestation of Strongly Correlated Electrons in a 2D Kagome Metal–Organic Framework, ADVANCED FUNCTIONAL MATERIALS, in press (2021), DOI: https://doi.org/10.1002/adfm.202106474.
88. Y. Huang, M. Shaibani, T. Gamot, M. Wang, P. Jovanović, D. Cooray, M. Mirshekarloo, R. Mulder, N. V. Medhekar, M. Hill and M. Majumder, A saccharide-based binder for efficient polysulfide regulations in Li-S batteries, NATURE COMMUNICATIONS 12, 1 (2021).
87. C. X. Trang, Q. Li, Y. Yin, J. Hwang, G. Akhgar, I. Bernardo, A. Grubišić-Čabo, A. Tadich, M. Fuhrer, S. Mo, N. V. Medhekar and M. Edmonds, Crossover from 2D Ferromagnetic Insulator to Wide Band Gap Quantum Anomalous Hall Insulator in Ultrathin $MnBi_2Te_4$, ACS NANO 15, 13444 (2021).
86. A. Kant, N. V. Medhekar and T. Bhandakkar, Spatial calcium kinetics after a traumatic brain injury, BIOMECHANICS AND MODELING IN MECHANOBIOLOGY 20, 1413 (2021).
85. A. Grubišić-Čabo, J. Kotsakidis, Y. Yin, A. Tadich, M. Haldon, S. Solari, I. Bernardo, K. Daniels, J. Riley, E. Huwald, M. Edmonds, R. Myers-Ward, N. V. Medhekar, D. Kurt Gaskill and Michael S Fuhrer, Magnesium-intercalated graphene on SiC: Highly n-doped air-stable bilayer graphene at extreme displacement fields, APPLIED SURFACE SCIENCE 541, 148612 (2021).
84. Y. Zhang, Y. Yin, G. Dubuis, T. Butler, N. V. Medhekar and S. Granville, Berry curvature origin of the thickness-dependent anomalous Hall effect in a ferromagnetic Weyl semimetal, NPJ QUANTUM MATERIALS 6, 1 (2021).
83. W. Yin, H. Li, A. Chesman, B.Tadgell, A. Scully, M. Wang, W. Huang, C. McNeill, W. Wong, N. V. Medhekar, P. Mulvaney and J. Jasieniak, Detection of halomethanes using cesium lead halide perovskite nanocrystals, ACS NANO 15, 1454 (2021).
82. S. Nanjunda, L. Zhou, Y. Yin, W. Yu, B. Shabbir, H. Mu, X. Bao, Y. Zhang, S. Tian, Q. Ou, S. Li, M. Hossain, Y. Zhang, H. Shao, G. Xing, N. V. Medhekar, C. Li, J. Liu and Q. Bao, Probing the dynamic structural changes of DNA using ultrafast laser pulse in graphene-based optofluidic device, INFOMAT 3, 316 (2021).

2020 [9 papers]

81. M. Wang, V. Vasudevan, S. Lin, J. Jasieniak, S. Russo, N. Birbilis and N. V. Medhekar, Molecular Mechanisms of Thermal Instability in Hybrid Perovskite Light Absorbers for Photovoltaic Solar Cells, JOURNAL OF MATERIALS CHEMISTRY A 8, 17765 (2020).
80. M. Fuhrer and N. V. Medhekar, Dirac-point photocurrents due to photothermoelectric effect in non-uniform graphene devices, NATURE NANOTECHNOLOGY 15 241, (2020).
79. J. C. Kotsakidis, A. Grubisič -Ćabo, Y. Yin, A. Tadich, R. L. Myers-Ward, M. DeJarld, S. P. Pavunny, M. Currie, K. M. Daniels, C. Liu, M. T. Edmonds, N. V. Medhekar, D. K. Gaskill, A. Vazquez de Parga´ and M. Fuhrer, Freestanding n-Doped Graphene via Intercalation of Calcium and Magnesium into the Buffer Layer−SiC(0001) Interface, CHEMISTRY OF MATERIALS 32, 6464 (2020).
78. Y. Wu, Q. Ou, Y. Yin, Y. Li, W. Ma, W. Yu, G. Liu, X. Cui, X. Bao, J. Duan, G. Álvarez-Pérez, Z. Dai, B. Shabbir, N. V. Medhekar, X. Li, C. Li, P. Alonso-González and Q. Bao, Chemical switching of low-loss phonon polaritons in α-MoO_3 by hydrogen intercalation, NATURE COMMUNICATIONS 11, 2646 (2020).
77. A. Varghese, D. Saha, K. Thakar, V. Jindal, S. Ghosh, N. V. Medhekar, S. Ghosh and S. Lodha, Near-Direct Bandgap WSe_2/ReS_2 Type-II pn Heterojunction for Enhanced Ultrafast Photodetection and High-Performance Photovoltaics, NANO LETTERS 20, 1707 (2020).
76. L. Bourgeois, Y. Zhang, Z. Zhang, Y. Chen and N. V. Medhekar, Transforming solid-state precipitates via excess vacancies, NATURE COMMUNICATIONS 11, 1248 (2020).
75. L. Li, M. Wang, J. Wang, F. Ye, S. Wang, Y. Xu, J. Liu, G. Xu, Y. Zhang, C. Yan, N. V. Medhekar, M. Liu and Y. Zhang, Asymmetric gel polymer electrolyte with high lithium ionic conductivity for dendrite-free lithium metal batteries, JOURNAL OF MATERIALS CHEMISTRY A 8, 8033 (2020).
74. N. Pai, J. Lu, M. Wang, A. Chesman, A. Seeber, P. Cherepanov, D. Senevirathna, T. Gengenbach, N. V. Medhekar, P. Andrews, U. Bach and A. Simonov, Enhancement of the intrinsic light harvesting capacity of $Cs_2AgBiBr_6$ double perovskite via modification with sulphide, JOURNAL OF MATERIALS CHEMISTRY A 8, 2008 (2020).
73. J. Collins, C. Wang, A. Tadich, Y. Yin, C. Zheng, J. Hellerstedt, A. Grubisic-Cabo, S. Tang, S. Mo, J. Riley, E. Huwald, N. V. Medhekar, M. Fuhrer and M. Edmonds, Electronic bandstructure of in-plane ferroelectric van der Waals β′-In_2Se_3, ACS APPLIED ELECTRONIC MATERIALS 2, 213 (2020).

2019 [10 papers]

72. V. Vasudevan, M. Wang, J. Yuwono, J. Jasieniak, N. Birbilis and N. V. Medhekar, Ion Agglomeration and Transport in $MgCl_2$-Based Electrolytes for Rechargeable Magnesium Batteries, JOURNAL OF PHYSICAL CHEMISTRY LETTERS 10, 7856 (2019).
71. Y. Yin, M. Fuhrer and N. V. Medhekar, Selective control of surface spin current in topological pyrite-type OsX_2 (X=Se, Te) crystals, NPJ QUANTUM MATERIALS 4, 1 (2019).
70. D. Kumar, C. Krull, Y. Yin, N. V. Medhekar and A. Schiffrin, Electric Field Control of Molecular Charge State in a Single-Component 2D Organic Nanoarray, ACS NANO 13, 11882 (2019)
69. M. Wang, J. Yuwono, V. Vasudevan, N. Birbilis and N. V. Medhekar, Atomistic mechanisms of Mg insertion reactions in group XIV anodes for Mg-ion batteries, ACS APPLIED MATERIALS AND INTERFACES 119, 774 (2019).
68. Z. Zhang, J. M. Rosalie, N. V. Medhekar and L. Bourgeois, Resolving the FCC/HCP interfaces of the (Ag_2Al) precipitate phase in aluminium, ACTA MATERIALIA 174, 116 (2019).
67. R. Deivanayagam, M. Cheng, M. Wang, V. Vasudevan, T. Foroozan, N. V. Medhekar and R. Shahbazian-Yassar, Composite Polymer Electrolyte for Highly Cyclable Room-Temperature Solid-State Magnesium Batteries, ACS APPLIED ENERGY MATERIALS 2, 7980 (2019).
66. A. Sharma, R. Babarao, N. V. Medhekar and A. Malani, Computational design of multilayer frameworks to achieve DOE target for on-board methane delivery, CARBON 152, 206 (2019).
65. J. Yuwono, N. Birbilis, C. Taylor, K. S. Williams, A. J. Samin and N. V. Medhekar, Aqueous electrochemistry of the magnesium surface: thermodynamic and kinetic profiles, CORROSION SCIENCE 147, 53 (2019).
64. F. Haque, A. Zavabeti, B. Zhang, R. Datta, Y. Yin, Z. Yi, Y. Wang, N. Mahmood, N. Pillai, N. Syed, H. Khan, A. Jannat, N. Wang, N. V. Medhekar, K. Kalantar-zadeh and J. Z. Ou, Ordered intercrystalline pores in planar molybdenum oxide for enhanced alkaline hydrogen evolution, JOURNAL OF MATERIALS CHEMISTRY A 7, 57 (2019).
63. B. Ananthoju, J. Mohapatra, D. Bahadur, N. V. Medhekar and A. Aslam, Influence of Cu_2ZnSnS_4 nanoparticles size on solar cell performance, SOLAR ENERGY MATERIALS AND SOLAR CELLS 189, 125 (2019).

2018 [8 papers]

62. M. Javadi, G. Simon and N. V. Medhekar, Atomistic insights into adsorption and stimuli-responsive behaviour of Poly (N-isopropylacrylamide)-Graphene hybrid systems, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 20, 28592 (2018).
61. Schiffrin, M. Capsoni, G. Farahi, C. Wang, C. Krull, M. Castelli, T. Roussy, K. Cochrane, Y. Yin, N. V. Medhekar, M. Fuhrer, A. Shaw, W. Ji and S. A. Burke, Designing optoelectronic properties by on-surface synthesis: formation and electronic structure of an Iron–Terpyridine macromolecular complex, ACS NANO 12, 6545 (2018).
60. Q. Ou, Z. Wang, J. Yuwono, Y. Zhang, R. Wang, Z. Dai, W. Li, C. Zheng, Z. Xu, X. Qi, S. Duhm, N. V. Medhekar, H. Zhang and Q. Bao, Strong depletion in hybrid perovskite p-n junctions induced by local electronic doping, ADVANCED MATERIALS 30, 1705792 (2018).
59. J. Mohapatra, B. Ananthoju, V. Nair, A. Mitra, D Bahadur, N. V. Medhekar and M Aslam, Enzymatic and non-enzymatic electrochemical glucose sensor based on carbon nano-onions, APPLIED SURFACE SCIENCE 442, 332 (2018).
59. A. Sharma, R. Babarao, N. V. Medhekar and A. Malani, Methane Adsorption and Separation in Slipped and Functionalized Covalent Organic Frameworks, INDUSTRIAL AND ENGINEERING CHEMISTRY RESEARCH 57, 4767 (2018).
58. P. D. White, S. A. Barter and N. V. Medhekar, Comparison of fatigue crack growth stress ratio effects under simple variable amplitude loading using fractographic and strain measurements, INTERNATIONAL JOURNAL OF FATIGUE 112, 240 (2018).
57. N. Alaal, N. V. Medhekar and A. Shukla, Tunable electronic properties of partially edge-hydrogenated armchair boron-nitrogen-carbon nanoribbons, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 20, 10345 (2018).
56. A. Kant, T. Bhandakkar and N. V. Medhekar, Stress enhanced calcium kinetics in a neuron, BIOMECHANICS AND MODELING IN MECHANOBIOLOGY 17, 169 (2018).

2017 [8]

55. J. Yuwono, N. Birbilis, R. Liu, Q. Ou, Q. Bao and N. V. Medhekar, Aqueous Electrochemical Activity of the Mg Surface: The Role of Group 14 and 15 Microalloying Elements, JOURNAL OF THE ELECTROCHEMICAL SOCIETY 164, C918 (2017).
54. Y. Yin, J. Cervenka and N. V. Medhekar, Molecular dipole driven electronic structure modifications of DNA/RNA nucleobases on graphene, JOURNAL OF PHYSICAL CHEMISTY LETTERS 8, 3087 (2017).
53. Y. Chen, Z. Zhang, N. V. Medhekar and L. Bourgeois, Vacancy-tuned precipitation pathways in $AlCu_{1.7}$ $In_{0.025}Sb_{0.025}$ (at.%) alloy, ACTA MATERIALIA 141, 341 (2017).
52. A. Sharma, A. Malani, N. V. Medhekar and R. Babarao, CO_2 Adsorption and Separation in Covalent Organic Frameworks with Interlayer Slipping, CRYSTENGCOMM 19, 6950 (2017).
51. J. Deng, Y. Yin, H. Niu, X. Ding, J. Sun and N. V. Medhekar, The edge stresses and phase transitions for magnetic BN

zigzag nanoribbons, SCIENTIFIC REPORTS 7, 7855 (2017).

50. Z. Zhang, J. Rosalie, J. Bourgeois and N. V. Medhekar, The bilayered precipitate phase ζ in the Al-Ag alloy system, ACTA MATERIALIA 132, 525 (2017).
49. N. Alaal, V. Loganathan, N. V. Medhekar and A. Shukla, From half-metal to semiconductor: electron correlation effects in zigzag SiC nanoribbons from first principles, PHYSICAL REVIEW APPLIED 7, 064009 (2017).
48. Y. Chen, Z. Zhang, Z. Chen, A. Tsalanidis, M. Weyland, S. Findlay, L. Allen, J. Li, N. V. Medhekar and L. Bourgeois, The enhanced theta-prime (θ′) precipitation in an Al-Cu alloy with trace Au additions, ACTA MATERIALIA 125, 340 (2017).

2016 [9 papers]

47. J. Yuwono, N. Birbilis, K.S. Williams and N. V. Medhekar, Electrochemical stability of magnesium surfaces in an aqueous environment, JOURNAL OF PHYSICAL CHEMISTRY C 120, 26922 (2016).
46. B. Ananthoju, J. Mohapatra, M. K. Jangid, D. Bahadur, N V. Medhekar and A. Aslam, Cation/Anion Substitution in Cu_2ZnSnS_4 for Improved Photovoltaic Performance, SCIENTIFIC REPORTS 6, 36369 (2016).
45. S. Thomas, N. Ott, R. Schaller, J. Yuwono, P. Volovitch, G. Sundararajan, N. V. Medhekar, K. Ogle, J. Scully and N. Birbilis, The effect of absorbed hydrogen on the dissolution of steel, HELIYON 2, e00209 (2016).
44. R. Huang, M. Hill, R. Babarao and N. V. Medhekar, CO_2 adsorption in azobenzene functionalized stimuli responsive metal–organic frameworks, JOURNAL OF PHYSICAL CHEMISTRY C 120, 16658 (2016).
43. Z. Zhang, T. Liu, A. E. Smith, N. V. Medhekar, P. Nakashima and L. Bourgeois, Mechanisms of void shrinkage in aluminium, JOURNAL OF APPLIED CRYSTALLOGRAPHY 49 (2016).
42. P. White, S. Barter and N. V. Medhekar, Hydrogen induced amorphisation around nanocracks in aluminium, ENGINEERING FRACTURE MECHANICS 161, 40 (2016).
41. L. Bourgeois, Z. Zhang, J. Li and N. V. Medhekar, The bulk and interfacial structure of η(Al_2Au) precipitate phase, ACTA MATERIALIA 105, 284 (2016).
40. J. van Embden, L. Bourgeois, E. Della Gaspera, L. Waddington, Y. Yin, N. V. Medhekar, J. Jasieniak and A. Chesman, The formation mechanism of Janus nanostructures in one-pot reactions: the case of Ag-Ag_8GeS_6, JOURNAL OF MATERIALS CHEMISTRY A 4, 7060 (2016).
39. N. Alaal, V. Loganathan, N. V. Medhekar and A. Shukla, First principles many-body calculations of electronic structure and optical properties of armchair SiC nanoribbons, JOURNAL OF PHYSICS D: APPLIED PHYSICS 49, 105306 (2016).

2015 [7 papers]

38. M. Mortazavi, Q. Ye, N. Birbilis and N. V. Medhekar, High capacity group-15 alloy anodes for Na-ion batteries: electrochemical and mechanical insights, JOURNAL OF POWER SOURCES 285, 29 (2015).
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APPENDIX A3. Invited/Keynote Talks and Presentations

27. N. V. Medhekar, (Invitation for Keyonote address) Global Summit and Expo on Graphene and 2D Materials, Edinburgh (Aug 2022).
26. N. V. Medhekar, Global Summit and Expo on Graphene and 2D Materials, Paris, France (Aug 2021), *delivered online*.
25. N. V. Medhekar, (Keynote address) International Conference on Nanomaterials and Atomaterial Sciences and Applications 2020, Melbourne (Feb 2020).
24. N. V. Medhekar, 20th International Union of Materials Research Societies conference, Perth (Sep 2019).
23. N. V. Medhekar, Pacific Rim Conference on Advanced Materials, Xi'an, China (Aug 2019).
22. N. V. Medhekar, 13th Annual International Electromaterials Science symposium, Geelong (Jan 2019).
21. N. V. Medhekar, International Conference on 2D Materials and Technologies, Melbourne, Australia (Dec 2018).
20. N. V. Medhekar, International Conference on Processing and Manufacturing of Advanced Materials Thermec, Paris, France (July 2018).
19. N. V. Medhekar, International Conference on Computational Engineering and Sciences, Funchal, Portugal (June 2017).
18. N. V. Medhekar, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'An, China (Dec 2016).
17. N. V. Medhekar, Department of Mechanical Engineering, National University of Singapore, Singapore (Sep 2015).
16. N. V. Medhekar, The Minerals, Metals and Materials Society (TMS) Annual Meeting, Orlando, Florida, USA (March 2015).
15. N. V. Medhekar, International Conference on Nanoscience and Nanotechnology, Adelaide, Australia (Feb 2014).
14. N. V. Medhekar, Sixth International Conference on Advanced Materials and Nanotechnology, Auckland, New Zealand (Feb. 2013).
13. N. V. Medhekar, International Conference on Emerging Advanced Nanomaterials, Brisbane, Australia (Oct 2012).
12. N. V. Medhekar, Molecular Modelling Workshop, Commonwealth Scientific and Industrial Research Organisation, Melbourne, Australia (June 2012).
11. N. V. Medhekar, AM-TCP Graphene Symposium, Commonwealth Scientific and Industrial Research Organisation, Melbourne, Australia (May 2012).
10. N. V. Medhekar, 35th Annual Condensed Matter and Materials Meeting, Wagga Wagga, Australia (Feb 2011).
9. N. V. Medhekar, Monash-Indian Institute of Technology joint research symposium, Mumbai, India (Feb 2011).
8. N. V. Medhekar, Research School of Physics and Engineering, Australian National University, Australia (Oct 2010).
7. N. V. Medhekar, School of Physics, University of Melbourne, Australia (Oct 2010).
6. N. V. Medhekar, Department of Mechanical Engineering, Johns Hopkins University, Baltimore, USA (March 2010).
5. N. V. Medhekar, Department of Mechanical Engineering, University of Colorado, Boulder, USA (March 2010).
4. N. V. Medhekar, Department of Mechanical Engineering, University of Notre Dame, USA (Feb 2010).
3. N. V. Medhekar, *Materials Research Society Meeting, Boston, USA (Dec 08).*
   *Recipient of the Materials Research Society's *Graduate Student Award.*
2. N. V. Medhekar, Yeshiva University, New York City, USA (Apr. 2008).
1. N. V. Medhekar, *McMAT ASME Applied Mechanics and Materials conference*, Austin, USA (June 2007).

APPENDIX A4. Research Supervision and Mentoring

Current research group members

Postdoctoral Researchers

1. Dr. Yuefeng Yin (2016–)
2. Dr. Hong Liu (2021–)

PhD Students (*Only students with the supervision load of at least 50% are listed here)*

1. Chutian Wang (thesis submitted, awaiting examiner reports)
2. Vallabh Vasudevan (thesis examination reports received with recommendation Pass with minor amendments, post-exam submission due by Nov 10, 2020)
3. Abin Varghese (IITB-Monash Research Academy student, 4th year)
4. Barnard Field (School of Physics, confirmation milestone completed in Feb 2020)
5 Victor Le (confirmation milestone completed in Feb 2020)
6. Madhav Sharma (commenced Jan 2021)
7. Ziyuan Zhao (commenced April 2021)
8. Enamul Haque (commenced April 2021)

Awards won by PhD students (current and alumni)

- Qile Li:
  - AINSE Postgraduate Research Award, The Australian Institute of Nuclear Science and Engineering (2020)
- Jodie Yuwono, graduated 2019:
  - Faculty of Engineering's GRITA award for overseas travel and collaboration (2017).
  - ***Monash University Vice Chancellor's Award for Thesis Excellence (2019).***
- Paul D. White, graduated 2020 (A mature-age, 60+ years old, worked part-time in industry whilst completing PhD):
  - DSTO cadetship award for PhD research (2017–2020).
- Zezhong Zhang, graduated 2018:
  - Young Scientist Award, International Conference on Aluminium Alloys (2016).
  - Best Poster Award, International Conference on Aluminium Alloys (2016).
- Yong Zhang, graduated 2018:
  - Student Scholar Award at the Conference of Microscopy and Microanalysis (2017).
- Runhong Huang, graduated 2015:
  - CSIRO top-up scholarship award $40K (2013).
- Majid Mortazavi, graduated 2015:
  - Overseas Travel Fellowship Award, Australian Nanotechnology Network (2015).

Research group alumni (and their employment status)

- Paul D. White (PhD student, 2015–2020, 0.5FTE), Defence Science and Technology, Melbourne.
- Zezhong Zhang (PhD student, 2015–2018), Postdoctoral Fellow jointly at the University of Antwerp, Belgium, and Oxford University, UK.
- Yong Zhang (PhD student, 2015–2018), Postdoctoral Fellow at Monash University.
- Jodie Yuwono (PhD student, 2015–2018), Postdoctoral Fellow at the University of New South Wales.
- Mahdi Javadi (PhD student 2016–2019), Postdoctoral Researcher at RMIT University.
- Aayush Kant (PhD student, 2016–2019), Postdoctoral Fellow at University of Pennsylvania, USA.
- Yiqing (Kelvin) Chen (Postdoctoral Fellow, 2016–2017), Postdoctoral Fellow at the Max Planck Institute of Iron Research, Dusseldorf, Germany.
- Naresh Alaal (PhD student at IITB–Monash Academy, 2013–2017), Postdoctoral Fellow at the King Abdulla University of Science and Technology, Saudi Arabia.
- Balakrishna Anathoju (PhD student at IITB–Monash Academy, 2012–2016), Postdoctoral Fellow at the University of Manchester, UK.
- Runhong Huang (PhD student, 2013–2016), Postdoctoral Fellow at the University of California, Irvine, USA.
- Majid Mortazavi (PhD student, 2012–2015), Postdoctoral Fellow at the Fritz Haber Institute of Max Planck Society, Berlin, Germany.
- Yuefeng Yin (PhD student, 2013–2016), Postdoctoral Fellow at Monash University.
- Dr. Junkai Deng (Postdoctoral Fellow, 2011–2013), Professor at Xi'an Jiaotong University, China.