

## Nikhil Medhekar

### Curriculum Vitae

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### Education

- 2009 Ph.D. (Mechanics of Solids and Structures), 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.  
2018– Deputy Associate Dean of Education (GPG), Faculty of Engineering, Monash University.

### Past Appointments

- 2010–2016 Senior Lecturer, Department of Materials Science & Engineering, Monash University.  
2015–2017 Director, Master of Advanced Engineering Course, Monash University.  
2008–2010 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 Silver Award for outstanding graduate research, Materials Research Society (USA).  
2008 William N. Findley Award for best research paper, Brown University.  
2002 Ashok Chaturvedi and P. M. Natu Memorial Awards for Outstanding Performance, Indian Institute of Technology, Bombay, India.  
2002 Nominated for Edison Engineering Development Program at General Electric Corporate Research.  
2000 Forbes Marshal Award for Best Undergraduate Thesis, University of Pune, India.

### Research

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 Monte Carlo methods, using massively parallel computing facilities.

### Grants and Research Support Summary

- ~\$33.4M in Australian Research Council's Funding, personal share ~\$2.7M.
- ~\$175K in Monash University intramural grants.

- 13M SUs in competitive National Computing Grants.
- ~\$120K in other research support.

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

### Research Output Summary

- More than 60 publications in top peer reviewed journals in materials science and engineering, including Advanced Materials, Nano Letters, ACS Nano, Journal of the American Chemical Society, Journal of Physical Chemistry Letters, Physical Review Letters and Acta Materialia.
- 15 invited conference presentations and talks.
- Total citations >2400 (Google Scholar), h-index 21.

*A full list of publications is available in the Appendix.*

### Current Research Group

- 10 PhD students, 8 as main supervisor.
- 2 postdoctoral researchers.
- 3 undergraduate researchers.

*See group's [webpage](#) for more information.*

### Research Group Alumni

- Yiqing (Kelvin) Chen (Postdoctoral Fellow, 2016–2017), currently Postdoctoral Fellow at Max Planck Institute of Iron Research, Dusseldorf, Germany.
- Naresh Alaal (PhD student at IITB–Monash Academy, 2013–2017), currently Postdoctoral Fellow at King Abdulla University of Science and Technology, Saudi Arabia.
- Bala Anathoju (PhD student at IITB–Monash Academy, 2012–2016), currently Postdoctoral Fellow at University of Manchester, UK.
- R. Huang (PhD student, 2013–2016), currently Postdoctoral Fellow at the University of California, Irvine, USA.
- M. Mortazavi (PhD student, 2012–2015), currently Postdoctoral Fellow at Fritz Haber Institute of Max Planck Society, Berlin, Germany.
- J. Deng (Postdoctoral Fellow, 2011–2013), currently Assistant Professor at Xi'an Jiaotong University, Xian, China.

### Service to Research Community

- Expert assessor for Australian Research Council's proposals (Discovery, Linkage Projects, DECRA and Future Fellowships), Austrian Research Fund, and Czech Republic Academy of Sciences.
- Chair, Pawsey High Performance Computing facility merit allocation committee (2017-2018).
- 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 assessor for masters and PhD theses (UNSW, RMIT).

### Teaching

- Modelling of Materials (2014, 2016).
- Materials Characterisation and Modelling (2011–2017).
- Structure Property Relationships in Materials (2011–2014).
- Materials Engineering Projects (2011–2018).

- Master of Advanced Engineering Research Projects (2016).

**Outreach**

- Several outreach activities in the wider community, promoting study and careers in science and technology. This was achieved via various platforms provided by the Tall Poppy Campaign, Australian Institute of Policy and Science, and University and Departmental outreach activities.
- As the chair of the departmental publicity committee, I regularly organise visits from high school students, immersion day, etc.

## APPENDIX

### Grants and Research Support

#### Australian Research Council (ARC) grants

2017–2023	M. Fuhrer, and 17 Chief Investigators including <u>N. V. Medhekar</u> . “Future Low Energy Electronics Technologies.” Centre of Excellence CE170100039.	\$33.4M
2016–2019	<u>N. V. Medhekar</u> , N. Birbilis and G. Williams. “Next Generation Batteries: Exploiting Divalent Magnesium.” Discovery Project DP160103661.	\$391K
2015–2017	L. Bourgeois and <u>N. V. Medhekar</u> . “Complex Interfaces and Solid-State Precipitation in Advanced Materials.” Discovery Project DP150100558.	\$374K
2013–2015	G. Simon, D. Li and <u>N. V. Medhekar</u> . “New Stimuli-Responsive Polymer Membranes using Graphene as a Multifunctional Scaffold.” Discovery Project DP130102512.	\$395K

#### Monash University Intramural 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, <u>N. V. Medhekar</u> , 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	<u>N. V. Medhekar</u> . “Discovering Non-Toxic Hybrid Perovskite Materials for High-Efficiency Solar Cells.” Monash University Faculty of Engineering Seed Grant.	\$20K
2014	<u>N. V. Medhekar</u> . “Porous Aromatic Frameworks for High Performance Energy Storage.” Monash University Faculty of Engineering Seed Grant.	\$30K
2013	<u>N. V. Medhekar</u> . “Next Generation Battery Materials.” Monash University Faculty of Engineering Seed Grant.	\$30K
2012	<u>N. V. Medhekar</u> . “High Performance Graphene Based Polymer Nanocomposites.” Monash University Faculty of Engineering Seed Grant.	\$30K
2011	<u>N. V. Medhekar</u> . “Understanding Mechanisms of Graphene Growth.” Monash University Faculty of Engineering Seed Grant.	\$10K
2011	<u>N. V. Medhekar</u> . Monash University Faculty of Engineering New Staff Member Grant.	\$8K

#### Nationally Competitive Computing grants

*Allocation of 1M Service Units (SUs) is monetarily equivalent to \$80K–\$100K.*

2019	<u>N. V. Medhekar</u> . “In Silico Design of Nanoscale Energy Materials.” Pawsey Energy and Resources Merit Allocation Grant.	3.5M SUs
2019	<u>N. V. Medhekar</u> . “Enabling Functional Properties of Nanomaterials using Atomistic Simulations.” National Computing Merit Allocation Grant.	1.5M SUs
2018	<u>N. V. Medhekar</u> . “In Silico Design of Nanoscale Energy Materials.” Pawsey Energy and Resources Merit Allocation Grant.	2.0M SUs
2018	<u>N. V. Medhekar</u> . “Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials.” National Computing Merit	3.5M SUs

	Allocation Grant.	
2017	<u>N. V. Medhekar</u> . "In Silico Design of Nanoscale Energy Materials." Pawsey Energy and Resources Merit Allocation Grant.	1.6M SU\$
2017	<u>N. V. Medhekar</u> . "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	2.0M SU\$
2016	<u>N. V. Medhekar</u> . "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	1.5M SU\$
2015	<u>N. V. Medhekar</u> . "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	1.0M SU\$
2014	<u>N. V. Medhekar</u> . "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	1.2M SU\$
2013	<u>N. V. Medhekar</u> . "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	1.2M SU\$
2012	<u>N. V. Medhekar</u> . "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	0.2M SU\$
2011	<u>N. V. Medhekar</u> . "Atomistic Simulations for Electronic, Chemical and Mechanical Properties of Nanomaterials." National Computing Merit Allocation Grant.	0.1M SU\$

1 Service Unit (SU) = 1 computer hour ~ \$0.10

### 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

## Publications

### Refereed Journal Papers

#### [2019]

67. Y. Yin, M. Fuhrer and N. V. Medhekar, Pyrite-type  $\text{OsX}_2$  (X=Se,Te) crystals: a novel topological material for selective control of surface spin current, arXiv: 1811.11330 (2019).
66. 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, arXiv: 1811.09032 (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  $\text{Cu}_2\text{ZnSnS}_4$  nanoparticles size on solar cell performance, SOLAR ENERGY MATERIALS AND SOLAR CELLS 189,

125 (2019).

### [2018]

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]

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 CHEMISTRY LETTERS* 8, 3087 (2017).
53. Y. Chen, Z. Zhang, N. V. Medhekar and L. Bourgeois, Vacancy-tuned precipitation pathways in AlCu<sub>1.7</sub>In<sub>0.025</sub>Sb<sub>0.025</sub> (at.%) alloy, *ACTA MATERIALIA* 141, 341 (2017).
52. A. Sharma, A. Malani, N. V. Medhekar and R. Babarao, CO<sub>2</sub> 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]**

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  $\text{Cu}_2\text{ZnSnS}_4$  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,  $\text{CO}_2$  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  $\eta(\text{Al}_2\text{Au})$  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  $\text{Ag-Ag}_8\text{GeS}_6$ , *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]**

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).
37. Y. Yin, J. Cervenka and N. V. Medhekar, Tunable Hybridization Between Electronic States of Graphene and Physisorbed Hexacene, *JOURNAL OF PHYSICAL CHEMISTRY C* 119, 19526 (2015).
36. A. Ahmed, R. Babarao, R. Huang, N. V. Medhekar, B. D. Todd, M. R. Hill and A. W. Thornton, Porous aromatic frameworks impregnated with lithiated fullerenes for natural gas purification, *JOURNAL OF PHYSICAL CHEMISTRY C* 119, 9347 (2015).
35. Y. M. Zhu, M. Weyland, N. V. Medhekar, C. Dwyer, C. L. Mendis, K. Hono and J. F. Nie, On the prismatic precipitate plates in Mg–Ca–In alloys, *SCRIPTA MATERIALIA* 101, 16 (2015).
34. Y. Wang, J. Z. Ou, A. Chrimes, B. Carey, T. Daeneke, M. M. Y. A. Alsaif, M. Mortazavi, S. Zhuiykov, N. V. Medhekar, M. Bhaskaran, J. Friend, M. Strano and K. Kalantar-Zadeh, Plasmon Resonances of Highly Doped Two-Dimensional  $\text{MoS}_2$ , *NANO LETTERS* 15, 883 (2015).
33. J. Cervenka, A. Budi, Ni. Dontschuk, A. Stacey, A. Tadich, K. Rietwyk, A. chen, M. Edmonds, Y. Yin, N. V. Medhekar, M. Kalbac and C. I. Pakes, Graphene field effect transistor as a probe of electronic structure and charge transfer at organic molecule-graphene interfaces, *NANOSCALE* 7, 1471 (2015).
32. S. Thomas, N. V. Medhekar, G. S. Frankel and N. Birbilis, Corrosion mechanism and hydrogen evolution on Mg, *CURRENT OPINION IN SOLID STATE AND MATERIALS SCIENCE* 19, 85 (2015).

**[2014]**

31. M. Mortazavi, C. Wang, J. Deng, V. B. Shenoy and N. V. Medhekar, Ab initio characterization of sodium intercalation in layered  $\text{MoS}_2$  for Na-ion batteries, *JOURNAL OF POWER SOURCES* 268, 279 (2014).

30. B. Ananthoju, F. Sonia, A. Kushawaha, D. Bahadur, N. V. Medhekar and M. Aslam, Improved structural and optical properties of  $\text{Cu}_2\text{ZnSnS}_4$  thin films, *ELECTROCHIMICA ACTA* 137, 154 (2014).
29. M. Y. A. Alsaif, K. Latham, M. R. Field, D. Yao, N. V. Medhekar, G. A. Beane, R. B. Kaner, S. Russo, J. Z. Ou and K. Kalantar-zadeh, Tunable plasmon resonance in two-dimensional molybdenum oxide nanoflakes, *ADVANCED MATERIALS* 26, 3931 (2014).

**[2013]**

28. R. Babarao, Y. Jiang and N. V. Medhekar, Post-combustion  $\text{CO}_2$  capture in functionalized porous coordination networks, *JOURNAL OF PHYSICAL CHEMISTRY C* 117, 26976 (2013).
27. L. Bourgeois, N. V. Medhekar, A. E. Smith, M. Weyland, J.-F. Nie and C. Dwyer, Efficient atomic-scale kinetics through a complex heterophase interface, *PHYSICAL REVIEW LETTERS* 111, 046102 (2013).
26. Y. Wang, J. Z. Ou, S. Balendhran, A. Chrimes, M. Mortazavi, M. R. Field, K. Latham, V. Bansal, J. Friend, S. Zhuiykov, N. V. Medhekar, M. S. Strano & K. Kalantar-zadeh, Electrochemical control of photoluminescence in two-dimensional  $\text{MoS}_2$  nanoflakes, *ACS NANO* 7, 10083 (2013).
25. J. Song, B. Ouyang and N. V. Medhekar, Energetics and kinetics of Li intercalation in irradiated hybridized graphene scaffolds, *ACS APPLIED MATERIALS AND INTERFACES* 5, 12968 (2013).
24. S. Balendhran, J. Deng, J. Z. Ou, J. Scott, J. Tang, K. L. Wang, S. Russo, S. Zhuiykov, M. S. Strano, N. V. Medhekar, S. Sriram, M. Bhaskaran and K. Kalantar-Zadeh, Enhanced charge carrier mobility in two-dimensional high dielectric molybdenum oxide, *ADVANCED MATERIALS* 25, 109 (2013).
23. M. Mortazavi, J. Deng, V. B. Shenoy and N. V. Medhekar, Elastic softening of alloy negative electrodes for Na-ion batteries, *JOURNAL OF POWER SOURCES* 225, 207 (2013).
22. J. Li, N. V. Medhekar and V. B. Shenoy, Bonding charge density and ultimate strength of monolayer transition metal dichalcogenides, *JOURNAL OF PHYSICAL CHEMISTRY C* 117, 15842 (2013).
21. J. Song and N. V. Medhekar, Thermal transport in lattice-constrained 2D hybrid graphene heterostructures, *JOURNAL OF PHYSICS: CONDENSED MATTER* 45, 445007 (2013).
20. J. Deng, J. Z. Liu and N. V. Medhekar, Enhanced lithium adsorption and diffusion on silicene nanoribbons, *RSC ADVANCES* 3, 20338 (2013).

**[2012]**

19. J. Deng, M. Mortazavi, N. V. Medhekar and J. Z. Liu, Band engineering for Ni-Mg-O alloys for photocathodes of high efficiency dye-sensitized solar cells, *JOURNAL OF APPLIED PHYSICS* 112, 123703 (2012).
18. J. Shang, G. Li, R. Singh, Q. Gu, K. M. Nairn, T. J. Bastow, N. V. Medhekar, C. M. Doherty, A. J. Hill, J. Z. Liu and P. A. Webley, Discriminative separation of gases by a "molecular trapdoor" mechanism in chabazite zeolites, *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY* 134, 19246 (2012).
17. J. Deng, I. Fampiou, J. Z. Liu, A. Ramasubramaniam and N. V. Medhekar, Edge stresses of non-stoichiometric edges in two-dimensional crystals, *APPLIED PHYSICS LETTERS* 100, 251906 (2012).
16. S. Chen, N. V. Medhekar, J. Garitaonandia and K. Suzuki, Surface charge transfer induced ferromagnetism in nanostructured ZnO/Al, *JOURNAL OF PHYSICAL CHEMISTRY C* 116, 8541 (2012).
15. N. Kirkland, T. Schiller, N. V. Medhekar and N. Birbilis, Exploring graphene as a corrosion protection barrier, *CORROSION SCIENCE* 56, 1 (2012).
14. S. Sriram, M. Bhaskaran, S. Chen, S. Jayawardhana, P. Stoddart, J. Z. Liu, N. V. Medhekar, K. Kalantar-Zadeh and A. Mitchell, Influence of electric field on SERS: frequency effects, intensity



changes and susceptible bonds, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 134 (10), 4646 (2012).

#### [2011 and prior]

13. N. V. Medhekar, A. Ramasubramaniam and V. B. Shenoy, Hydrogen bond networks in graphene oxide composites: structure and mechanical properties, ACS NANO 4, 2300 (2010).
12. A. Bagri, R. Grantab, N. V. Medhekar and V. B. Shenoy, Stability and formation mechanisms of carbonyl- and hydroxyl-decorated holes in graphene oxide, JOURNAL OF PHYSICAL CHEMISTRY C 114, 12053 (2010).
11. M. Z. Hossain, N. V. Medhekar, V. B. Shenoy and H. T. Johnson, Enhanced quantum confinement due to nonuniform composition in alloy quantum dots, NANOTECHNOLOGY 21, 095401 (2010).
10. J. B. Hannon, R. M. Tromp, N. V. Medhekar and V. B. Shenoy, Spontaneous formation and growth of a new polytype on SiC(0001), PHYSICAL REVIEW LETTERS 103, 256101 (2009).
9. N. V. Medhekar, V. Hegadekotte and V. B. Shenoy, Composition maps in coherent and dislocated alloy nanocrystals, SOLID STATE COMMUNICATIONS 149, 1395 (2009).
8. A. Ramasubramaniam, N. V. Medhekar and V. B. Shenoy, Substrate-induced magnetism in epitaxial graphene buffer layers, NANOTECHNOLOGY 20, 275705 (2009).
7. N. V. Medhekar, V. B. Shenoy, W. L. Chan and E. Chason, Stress-enhanced pattern formation on surfaces during low-energy ion bombardment, JOURNAL OF PHYSICS: CONDENSED MATTER 21, 224021 (2009).
6. N. V. Medhekar, V. Hegadekotte and V. B. Shenoy, Composition maps in self-assembled alloy quantum dots, PHYSICAL REVIEW LETTERS 100, 106104 (2008).
5. H. Ramanarayan, N. V. Medhekar and V. B. Shenoy, Microstructural evolution of strained heteroepitaxial multilayers, APPLIED PHYSICS LETTERS 92, 173107 (2008).
4. N. V. Medhekar and V. B. Shenoy, Shape dynamics in anisotropically strained 2D self-assembling systems, JOURNAL OF APPLIED PHYSICS 103, 063523 (2008).
3. N. V. Medhekar, V. B. Shenoy, J. B. Hannon and R. M. Tromp, Self-assembling surface stress domains far from equilibrium, APPLIED PHYSICS LETTERS 91, 253101 (2007).
2. N. V. Medhekar, V. B. Shenoy, J. B. Hannon and R. M. Tromp, Metastability in 2D self-assembling systems, PHYSICAL REVIEW LETTERS 99, 156102 (2007).
1. N. V. Medhekar and S. K. Maiti, Derivative procedure for BEM based computation of change in natural frequency, INTERNATIONAL JOURNAL OF FRACTURE 118(3), L51 (2002).

#### Refereed Conference Papers

2. J. Deng, J. Z. Liu and N. V. Medhekar, Non-equivalent zigzag edge stresses for 2D binary compound nanoribbons, Proceedings of IEEE 2012 conference on Optoelectronic and Microelectronic Materials and Devices 1, 65 (2012).
1. N. V. Medhekar, Non-uniform composition distribution in alloy quantum structures, Proceedings of IEEE 2010 conference on Optoelectronic and Microelectronic Materials and Devices 1, 175 (2010).

#### Invited Presentations and Talks

15. N. V. Medhekar, International Conference on 2D Materials and Technologies, Melbourne, Australia (Dec 2018).
14. N. V. Medhekar, International Conference on Processing and Manufacturing of Advanced Materials Thermec, Paris, France (July 2018).

13. N. V. Medhekar, International Conference on Computational Engineering and Sciences, Funchal, Portugal (June 2017).
12. N. V. Medhekar, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an, China (Dec 2016).
11. N. V. Medhekar, The Minerals, Metals and Materials Society (TMS) Annual Meeting, Orlando, Florida, USA (March 2015).
10. N. V. Medhekar, International Conference on Nanoscience and Nanotechnology, Adelaide, Australia (Feb. 2014).
9. N. V. Medhekar, Sixth International Conference on Advanced Materials and Nanotechnology, Auckland, New Zealand (Feb. 2013).
8. N. V. Medhekar, International Conference on Emerging Advanced Nanomaterials, Brisbane, Australia (Oct. 2012).
7. N. V. Medhekar, Molecular Modelling Workshop, Commonwealth Scientific and Industrial Research Organisation, Melbourne, Australia (June 2012).
6. N. V. Medhekar, AM-TCP Graphene Symposium, Commonwealth Scientific and Industrial Research Organisation, Melbourne, Australia (May 2012).
5. N. V. Medhekar, 35<sup>th</sup> Annual Condensed Matter and Materials Meeting, Wagga Wagga, Australia (Feb. 2011).
4. N. V. Medhekar, Monash-Indian Institute of Technology research symposium, Mumbai, India (Feb. 2011).
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)*.