

Nitin Shriram Wadnerkar

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EDUCATION

Doctor of Philosophy, Physics
Swami Ramanand Teerth Marathwada University, Nanded, Maharashtra, India 2011
THESIS - 'Computational study of organometallic compounds and their hydrogen uptake'

Master of Science, Physics
Swami Ramanand Teerth Marathwada University, Nanded, Maharashtra, India 2005

Bachelor of Science, Physics, Chemistry, and Computer Science
Swami Ramanand Teerth Marathwada University, Nanded, Maharashtra, India 2003

PROFESSIONAL EXPERIENCE

PCET's Pimpri Chinchwad University, Sate, Maval, Pune, Maharashtra, India
(School of Engineering & Technology) 2023 – till date
Assistant Professor

- Subjects Taught: Quantum Mechanics, Nanotechnology, Semiconductor Physics, Computational Physics.

University of Ostrava, Ostrava, Czech Republic 2020 – 2021
Senior Postdoc Researcher

- Physics of nanostructures, structural, optical and electronic properties of 2D materials.

Linköping University, Norrköping, Sweden 2017 – 2019
Postdoctoral Research Fellow

- Studies of organic energy devices and related materials, their utilization for hydrogen storage, hydrogen peroxide generation, supercapacitance applications, and applications for the fuel cell technology.

Indian Insitute of Science Education and Research, Pune, Maharashtra, India 2014 – 2017
Postdoctoral Research Fellow

- Studies of perovskite surfaces and oxygen reduction mechanisms thereon for fuel cell application.; Structural, optical, and electronic properties of quarternary chalcogenides as a solar cell absorbers.

University College Dublin, Dublin, Ireland 2012 – 2013
Research Engineer

- Worked on the science foundation Ireland funded project entitled 'Doping of Titania and metal oxides for photovoltaic materials design'.; Modelling of electronic structure of metal oxides.; Modelling surfaces of the items above, examination of hydrated metal oxide surfaces and their dynamical properties

Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan 2011
Exchange student

- Worked on the project entitled 'Ab-initio multi-scale study of proton transfer and solvation in water clusters'.

Swami Ramanand Teerth Marathwada University, Nanded, Maharashtra, India 2008 – 2011
Senior Research Fellow at PhD level

- Worked on a project entitled 'Computational study of hydrogen storage capacity of organometallic compounds using density functional methods' funded by CSIR, New Delhi, India.

AWARD, RECOGNITION, AND OTHER RESPONSIBILITIES

- **Course Coordinator - Engineering Physics**, Pimpri Chinchwad University, Sate, Maval , Pune (2023-till date)
- **Member, Course Development Review Committee - Engineering Physics**, Pimpri Chinchwad University, Sate, Maval, Pune (2023-till date)
- **Member, Board of Studies**, Pimpri Chinchwad University, Sate, Maval, Pune (2023-till date)
- **Member, Board of Exam**, Pimpri Chinchwad University, Sate, Maval, Pune (2023-2024)
- **'Best Poster Award'** in international conference "Advanced Functional Materials-2018", Sweden
- **Reviewer**: high impact journals in Elsevier, Royal Society of Chemistry, SpringerNature journals

GRANTS (Principal Investigator)

2020-2021: CPU time: IT4Innovations National Supercomputing Centre (within Czech Republic and Europe), Open Access calls (1.2M corehours in total)

RESEARCH SKILLS

- DFT and MP2 theory, Atom-Density Matrix Propagation simulations, reaction kinetics of molecules/polymers (GAUSSIAN package)
- Periodic, plane-wave Density functional theory (VASP, Quantum Espresso softwares)
- Periodic, symmetry-adjusted DFT (CRYSTAL code)
- Force field generation and ab initio molecular dynamics simulations (GROMACS)
- GPAW: DFT and beyond within the projector-augmented wave method
- Computation of structural, electronic, optical properties of 0D, 2D, 3D materials
- Modelling surfaces of the item above, examination of hydrated metal oxide surfaces
- Oxygen reduction reactions on transition metal perovskite surfaces (with/without Jahn-Teller effect) for fuel cell application
- Organic polymers/semiconductors for energy applications
- Worked on observational facility, 'Giant Meter wave Radio Telescope (GMRT)' for radio astronomical research in meter wavelengths range of radio spectrum (it is located at a site about 80 km north of Pune, India), during 2006-2008.
- Data Analysis with NRAO AIPS (Astronomical Image Processing System) as well as Imaging, Photometry with IRAF (Image Reduction and Analysis Facility).

PUBLICATIONS

Total (published)	26 (Refereed journals = 24 and Conference proceedings = 2)
First/Corresponding authors	14
Total citations	730+
h index	16

SCOPUS ID: <http://www.scopus.com/authid/detail.uri?authorId=35090690700>

ORCID: <https://orcid.org/0000-0002-8444-0948>

- **Nitin Wadnerkar**, Niall English. Dynamical properties of oxygen-adsorbed LaMnO₃ perovskite surfaces at ambient and solid oxide fuel cells' operating temperature. ??, under preparation
- Soumalya Kaluva, Bhagvat Kharat, **Nitin Wadnerkar**, and Mahadevappa Nagnathappa. DFT and TD-DFT Study of Many-body and Hydrogen Bonding interactions: Nitrosamine Oligomers. *ChemistrySelect*, 9(18):e202303885, 2024

- **Nitin Wadnerkar**, Viktor Gueskine, Eric Glowacki, and Igor Zozoulenko. DFT Mechanistic Study on H₂O₂ Production using an Organic Semiconductor Epindolidione. *Journal of Physical Chemistry A*, 124(46):9605–9610, 2020
- **Nitin Wadnerkar**, Magnus Berggren, and Igor Zozoulenko. Exploring hydrogen storage in PEDOT: A computational study. *The Journal of Physical Chemistry C*, 123(4):2066–2074, 2019
- Sachin Rondiya, **Nitin Wadnerkar**, Yogesh Jadhav, Sandesh Jadkar, Santosh Haram, and Mukul Kabir. Structural, electronic, and optical properties of Cu₂NiSnS₄: a combined experimental and theoretical study toward photovoltaic applications. *Chemistry of Materials*, 29(7):3133–3142, 2017
- Niall J English, Mahfujur Rahman, **Nitin Wadnerkar**, and JMD MacElroy. Photo-active and dynamical properties of hematite (Fe₂O₃)–water interfaces: an experimental and theoretical study. *Physical Chemistry Chemical Physics*, 16(28):14445–14454, 2014
- Mahfujur Rahman, **Nitin Wadnerkar**, Niall J English, and JMD MacElroy. The influence of ti- and si-doping on the structure, morphology and photo-response properties of α -Fe₂O₃ for efficient water-splitting: Insights from experiment and first-principles calculations. *Chemical Physics Letters*, 592:242–246, 2014
- Kevin A McDonnell, **Nitin Wadnerkar**, Niall J English, Mahfujur Rahman, and Denis Dowling. Photo-active and optical properties of bismuth ferrite (BiFeO₃): an experimental and theoretical study. *Chemical Physics Letters*, 572:78–84, 2013
- **Nitin Wadnerkar** and Niall J English. Density functional theory investigations of bismuth vanadate: Effect of hybrid functionals. *Computational Materials Science*, 74:33–39, 2013
- Vijayanand Kalamse, **Nitin Wadnerkar**, and Ajay Chaudhari. Multi-functionalized naphthalene complexes for hydrogen storage. *Energy*, 49:469–474, 2013
- **Nitin Wadnerkar**, Vijayanand Kalamse, and Ajay Chaudhari. Hydrogen adsorption on C₃H₃–TM (TM= Sc, Ti) organometallic compounds. *Structural Chemistry*, 24(2):369–374, 2013
- **Nitin Wadnerkar**, Vijayanand Kalamse, and Ajay Chaudhari. Can ionization induce an enhancement of hydrogen storage in Ti₂–C₂H₄ complexes? *RSC Advances*, 2(22):8497–8501, 2012
- Vijayanand Kalamse, **Nitin Wadnerkar**, Amol Deshmukh, and Ajay Chaudhari. Interaction of molecular hydrogen with ni doped ethylene and acetylene complex. *International Journal of Hydrogen Energy*, 37(6):5114–5121, 2012
- Vijayanand Kalamse, **Nitin Wadnerkar**, and Ajay Chaudhari. Hydrogen storage in C₃Ti complex using quantum chemical methods and molecular dynamics simulations. *Journal of Molecular Modeling*, 18(6):2423–2431, 2012
- **Nitin Wadnerkar**, Vijayanand Kalamse, Shyi-Long Lee, and Ajay Chaudhari. Verification of dft-predicted hydrogen storage capacity of VC₃H₃ complex using molecular dynamics simulations. *Journal of Computational Chemistry*, 33(2):170–174, 2012
- Vijayanand Kalamse, **Nitin Wadnerkar**, Amol Deshmukh, and Ajay Chaudhari. C₂H₂M (M= Ti, Li) complex: a possible hydrogen storage material. *International Journal of Hydrogen Energy*, 37(4):3727–3732, 2012
- **Nitin Wadnerkar**, Vijayanand Kalamse, AB Phillips, BS Shivaram, and Ajay Chaudhari. Vibrational spectra of Ti:C₂H₄(nH₂) and Ti:C₂H₄(nD₂)(n= 1–5) complexes and the equilibrium isotope effect: calculations and experiment. *International Journal of Hydrogen Energy*, 36(16):9727–9732, 2011
- **Nitin Wadnerkar**, Vijayanand Kalamse, and Ajay Chaudhari. VC₃H₃ organometallic compound: a possible hydrogen storage material. *International Journal of Hydrogen Energy*, 36(1):664–670, 2011
- Vijayanand Kalamse, **Nitin Wadnerkar**, and Ajay Chaudhari. Theoretical study of third-row transition metal monofluorides. *International Journal of Quantum Chemistry*, 111(9):2014–2020, 2011
- **Nitin Wadnerkar**, Vijayanand Kalamse, and Ajay Chaudhari. Hydrogen storage in neutral and charged metalized-C_nH_m (for n= m and n \neq m) compounds. In *Nanotechnology (IEEE-NANO), 2010 10th IEEE Conference on*, pages 773–776. IEEE, 2010

- **Nitin Wadnerkar**, Vijayanand Kalamse, and Ajay Chaudhari. Hydrogen uptake capacity of C_2H_4Sc and its ions: a density functional study. *Journal of Computational Chemistry*, 31(8):1656–1661, 2010
- **Nitin Wadnerkar**, Vijayanand Kalamse, and Ajay Chaudhari. Higher hydrogen uptake capacity of $C_2H_4Ti^+$ than C_2H_4Ti : a quantum chemical study. *Theoretical Chemistry Accounts*, 127(4):285–292, 2010
- Vijayanand Kalamse, **Nitin Wadnerkar**, and Ajay Chaudhari. Hydrogen storage in C_2H_4V and $C_2H_4V^+$ organometallic compounds. *The Journal of Physical Chemistry C*, 114(10):4704–4709, 2010
- Vijayanand Kalamse, **Nitin Wadnerkar**, and Ajay Chaudhari. Quantum chemical study of dissociation of H_2 on C_3H_3V organometallic compound. *International Journal of Quantum Chemistry*, 110(10):1947–1952, 2010
- J. Bagchi, J. Jacob, Gopal-Krishna, Nitin Wadnerkar, J. Belapure, N. Werner, and A. C. Kumbharkhane. Diffuse Bubble-Like Radio-Halo Emission in MRC 0116+111: Imprint of AGN Feedback in a Distant Cluster of Galaxies. In D. J. Saikia, D. A. Green, Y. Gupta, and T. Venturi, editors, *The Low-Frequency Radio Universe*, volume 407 of *Astronomical Society of the Pacific Conference Series*, page 255, September 2009
- Joydeep Bagchi, Joe Jacob, Gopal-Krishna, Norbert Werner, **Nitin Wadnerkar**, Jaydeep Belapure, and A. C. Kumbharkhane. A diffuse bubble-like radio-halo source MRC 0116+111: imprint of AGN feedback in a low-mass cluster of galaxies. *Monthly Notices of the Royal Astronomical Society*, 399(2):601–614, 2009

BOOK CHAPTER

- **Nitin Wadnerkar**, V.G. Kalamse, and Ajay Chaudhari. Organometallic nanostructures: Hydrogen storage, structure stability and kinetics. In James C. Taylor, editor, *Advances in Chemistry Research*, chapter 6, pages 157–205. Nova Science Publisher Inc. New York, 2015

CONFERENCE/WORKSHOP/SCHOOL/MEET

Oral:

- Hydrogen storage in neutral and charged metalized- C_nH_m (for $n=m$ and $n \neq m$) compounds in 10th International Conference on Nanotechnology; Joint Symposium with NANO Korea 2010, KINTEXT, Seoul, South Korea, in August 17-20, 2010.

Posters:

- ‘Exploring the hydrogen storage in poly(3,4-ethylenedioxythiophene) (PEDOT) organic polymer’, received **Best Poster Award** in the international conference ‘Advanced Functional Materials-2018’, Kolmården, Sweden in August 21-23, 2018.
- ‘Can ionization induce an enhancement of hydrogen storage in $Ti_2-C_2H_4$ complex?’ in the 1st International Conference on Physics of Materials and Materials based Device Fabrication, organized by Department of Physics, Shivaji University, Kolhapur, India, in January 17-19, 2012.
- ‘Hydrogen storage in transition metal–decorated organic molecules’ in International Conference on Nanoscience and Nanotechnology at Swami Ramanand Teerth Marathwada University, Nanded, India in January 11-13, 2011.
- ‘Quantum chemical study of hydrogen storage capacity of nanomaterials’ Received **2nd prize** in 3rd student research convention Anvenshan-2010, Organized by N. E. S. College, Nanded and jointly sponsored by association of Indian Universities, New Delhi and Swami Ramanand Teerth Marathwada University, Nanded, India, in November 23-24, 2009.
- ‘Theoretical investigation of hydrogen storage capacity of organometallic compounds’, International conference on Hydrogen and Hydrogen storage; Methods and Materials, IISc, Bangalore, India, in January 3-6, 2009.

- 'GMRT Continuum Study of Star forming Regions S64 and S158' in Young Astronomers' Meet at Mahatma Gandhi University, Kottayam, Kerala, India.

Participations:

- Workshop, '8th USPEX workshop' at Shiv Nadar University, Gautam Budhha Nagar, Noida, India, in January 20-24, 2015.
- A school on 'Ab Initio Modeling in Solid State Chemistry MSSC-2012 at Imperial College London, London (UK) in September 17-21, 2012.
- Workshop on 'Galaxies: Normal and Active' at School of Physical of Sciences, Jointly organized with Inter-University Centre for Astronomy and Astrophysics (IUCAA), Pune, India, in November 14-17, 2011
- Workshop on 'Dynamics and Structure of Water: From Gas Phase Clusters to Condensed Phase', at Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, in October 13-16, 2011.
- 11th Workshop on First-Principles Computational Materials Physics, organized by focus group on computational materials research at Sun Moon lake Youth Activity Centre, Taiwan, in August 7-9, 2011.
- Co-authored Oral: 'C₂H₂M (M=Ti, Li) complex: a possible hydrogen storage material' in International Conference on Renewable Energy at University of Rajasthan, Jaipur, India, in January 17-21, 2011.
- Advances in Computer Aided Drug Designing organized by School of Life Sciences, Swami Ramanand Teerth Marathwada University, Nanded and School of Technology, Swami Ramanand Teerth Marathwada University Sub-Centre, Latur with VLife Science Technologies Pvt. Ltd. Pune, India, in February 18, 2010
- Co-authored Poster: 'Ti-C_x (x=2-3) and Ti₂-C₂ nanoclusters for hydrogen storage', International Conference on Advanced Nanomaterials and Nanotechnology at IIT, Guwahati, India, in December 9-11, 2009.
- Co-authored Oral: 'Diffuse bubble-like radio-halo emission in MRC 0116+111: a 'fossil' remnant of AGN feedback in a distant cluster of galaxies' in an international conference 'Low Frequency Radio Universe at NCRA, Pune, India, in December 8-12, 2008.
- Virtual Observatory workshop at IUCAA, Pune, India, in October 14-19, 2007.
- Completed a project titled, 'Spectra and Interpretation of Galactic Sources' in Radio Astronomy School 2007 under supervision of Prof. A. P. Rao, NCRA, Pune, India.

RESEARCH VISITS

IUCAA and TIFR-NCRA, Pune, India (2005-2008); University of Cantabria, Santander, Spain (June 8-12, 2012)

SCIENTIFIC/TECHNICAL SKILLS

Operating systems: Windows, Linux; Languages: FORTRAN, C, Python
Packages (Data science): Numpy, Scipy, Pandas, Matplotlib, Plot.ly, Tableau
Statistics/ML: Linear/Logistic regression, Ensemble trees, Random Forests, Clustering

REFERENCES

1. Prof. Dr. Ajay S. Chaudhari

(PhD Supervisor) Professor and Head,
Department of Physics, The Institute of Science,
Fort, Mumbai – 400 032, Maharashtra, India.
e-mail: ajaychau5@yahoo.com

2. Prof. Dr. Niall J. English

(PostDoc mentor) Professor,
School of Chemical and Bioprocess Engineering,
University College Dublin, Belfield, Dublin 4, Ireland.
e-mail: niall.english@ucd.ie