



## FACULTY PROFILE

**Name:** Dr. Nidhi Vyas

**Designation:** Assistant Professor

**E-Mail:** nidhivyas12@gmail.com, nidhiv@srmist.edu.in

**Orchid Id:** 0000-0003-0669-9003

➤ **Work Experience:** 8 Years in R & D

➤ **Professional Qualification:**

Degree	Institute/University	Specialization	Year of Passing
Ph.D.	Motilal Nehru National Institute of Technology(MNNIT), Allahabad(U.P.)	Physics	2011
M.Sc.	Bundelkhand University(B.U.)Jhansi	Physics (Condensed Matter Physics)	2006
B.Sc.	D.V.C. Orai (B.U. Jhansi)	Physics, Chemistry, Maths	2004

➤ **Research Interest:**

1. Modelling bio-inspired catalytic reactions
2. Molecular Magnet
3. Computational and spectroscopic study of biomolecules

➤ **Publications (Journals & Conferences):**

1. Aditya Kumar; Saurav Kumar Ojha; **Nidhi Vyas**, Animesh Ojha"(2022) Light and stable LinB14 (n=1-5) clusters for high capacity hydrogen storage at room temperature: A DFT study" **International Journal of Hydrogen Energy**, 47, 7861-7869
2. Vikrant Singh Rajput,#, Ritika Sharma,#, Anchala Kumari#, **Nidhi Vyas**, Vijay Prajapati and Abhinav Grover (2022)"Engineering a Multi Epitope Vaccine Against SARS-CoV-2 By Exploiting Its Non Structural and Structural Proteins" **Journal of Biomolecular Structure and Dynamics**, 40, 9096-9113
3. **Nidhi Vyas**, Asmita Sen, Aditya Kumar, Abhinav Grover (2021)"Computational study of ammonia generation by iron(III) and iron(IV) complexes bearing TPB ligand" **International Journal of Quantum Chemistry**, 121, e26775
4. Aditya Kumar, Saurav Kumar Ojha, **Nidhi Vyas.**, Animesh Ojha (2021) "Designing organic electron transport layers for stable and efficient performance of perovskite solar cells : A Theoretical Study" **ACS Omega** 6,7086-7093.
5. Asmita Sen<sup>#</sup>, **Nidhi Vyas**<sup>#</sup>, Bhawana Pandey, , Gopalan Rajaraman (2020) "Deciphering the Mechanism of

- Oxygen Atom Transfer by Non-heme Mn<sup>IV</sup>-Oxo Species: An Ab initio and DFT Exploration" *Dalton Transactions*, 49, 10380 -10393 (HOT Article).
6. Aditya Kumar, **Nidhi Vyas**, Animesh Ojha (2020) " Hydrogen Storage in Magnesium Decorated Boron Clusters (Mg<sub>2</sub>B<sub>n</sub>, n=4-14): A Density Functional Theory Study" *International Journal of Hydrogen Energy*, 45,12961-12971
  7. **Nidhi Vyas**, Aditya Kumar, Animesh K Ojha, Abhinav Grover, (2020) "Electronic Structure of iron dinitrogen complex [(TPB)FeN<sub>2</sub>]<sup>2-/1/0</sup>:correlation to Mössbauer parameters" *RSC Advances*, 10,7948 - 7955.
  8. Asmita Sen #, **Nidhi Vyas**#, Bhawana Pandey, Madhavan Jaccob, Gopalan Rajaraman, (2020) " Mechanistic Insights on the Formation of Mn<sup>III/IV</sup>=O Species Using Oxygen: A Theoretical Perspective" *Israel Journal of Chemistry* 60, 1–15
  9. **Nidhi Vyas**, Bhawana Pandey, Animesh K. Ojha, AbhinavGrover, (2019) "Revisiting Mechanistic Studies on Dinitrogen Reduction to Ammonia by an Iron Dinitrogen Complex as Nitrogenase Mimic" *International Journal of Quantum Chemistry* 119, 1-12.
  10. Snehasis Bhunia , Stefan Foster, **Nidhi Vyas**, Hans-Christian Schmitt, Animesh K. Ojha (2015) "Direct visual evidence for end-on adsorption geometry of Py on silver surface investigated by surface enhanced Raman scattering and density functional theory calculations" *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*151, 888-894.
  11. Bhawana Pandey, Azaj Ansari, Nidhi Vyas, Gopalan Rajaraman (2015) "Structures, Bonding and Reactivity of Iron and Manganese High-valent Metal-oxo Complexes: A Computational Investigation." *Journal of Chemical Science*, 127, 343–352.
  12. Jamie M Frost, Robert J Stirling, Sergio Sanz, **Nidhi Vyas**, Gary S Nichol, Gopalan Rajaraman, Euan K Brechin (2015) Turning a "useless" ligand into a "useful" ligand: a magneto-structural study of an unusual family of CuII wheels derived from functionalised phenolic oximes. *Dalton Transaction*, 44, 10177-10187
  13. Mursaleem Ansari, **Nidhi Vyas**, Azaj Ansari, Gopalan Rajaraman (2015)"Oxidation of Methane by an N-bridged High-Valent diiron-Oxo Species: Electronic Structure Implications to the Reactivity" *Dalton Transaction* 44,15232-15243
  14. Snehasis Bhunia, **Nidhi Vyas**, Chandan Sahu, Animesh K Ojha (2014) "Size Dependent Structural, Electronic and Magnetic Properties of ScN (N=2-14) Clusters Investigated by Density Functional Theory" *Journal of Molecular Modeling*, 20, 2481-2495
  15. Animesh K. Ojha, **Nidhi Vyas**, , Satya. P. Dubey, (2012) "Gas phase structural stability of neutral and zwitterionic forms of alanine in presence of (Water)<sub>n</sub>=1-7 Clusters: A density functional theory Study. *Computational and Theoretical Chemistry*, 1002, 16-23
  16. **Nidhi Vyas**, Animesh K. Ojha (2012) "Interaction of gold nano clusters of different size with adenine: A density functional study of neutral, cationic and anionic forms of [adenine + (Au)<sub>n=3, 6, 9, 12</sub>] complexes." *Computational and Theoretical Chemistry*, 984, 93-101.
  17. Susmita Bhattacharya, **Nidhi Vyas**, Animesh K Ojha, Swagata Dasgupta, Anushree Roy (2012) "Surface-enhanced Raman measurements and DFT calculations for l-tryptophan of varying pH in silver sol." *Journal of Raman Spectroscopy*, 43, 718-723.
  18. **Nidhi Vyas**, Animesh K. Ojha (2012) "Investigation on transition states of different stable conformers of [Alanine + M]<sup>++</sup> (M = Ca<sup>++</sup>, Cu<sup>++</sup> and Zn<sup>++</sup>) complexes: A quantum chemical study." *International Journal of Quantum Chemistry*, 112, 1526-1536.
  19. Manish Srivastava, **Nidhi Vyas**, Animesh. K. Ojha.. (2011) "Size dependent electron-phonon coupling in Li<sub>0.5</sub>Co<sub>0.1</sub>Fe<sub>2.4</sub>O<sub>4</sub> nanoparticles investigated by Raman spectroscopy". *Vibrational Spectroscopy*, 56, 19-25.
  20. **Nidhi Vyas**, Animesh K. Ojha, Arnulf Materny (2011) "Simulation of the Raman spectra of zwitterionic glycine + nH<sub>2</sub>O (n=1,2...5) by means of DFT calculations and comparison to the experimentally observed Raman spectra of glycine in aqueous medium" *Vibrational Spectroscopy*, 55, 69-76.
  21. **Nidhi Vyas**, Animesh K. Ojha (2011) "Calculation of dissociation constants and chemical hardness of some biologically important molecules: A theoretical study" *International Journal of Quantum Chemistry*, 111, 3961-

3970.

22. **Nidhi Vyas**, Animesh K. Ojha (2011) "A study on interaction of  $Be^{++}$ ,  $Mg^{++}$  and  $Ca^{++}$  with phenylalanine: binding energies, metal ion affinities and IR signature of complex stability". **Vibrational Spectroscopy**, 56, 42-50.
23. **Nidhi Vyas**, Animesh K. Ojha, (2011) "Effect of regular hydration on gas phase structural stability of [Zwitterionic Alanine +  $M^+$ ] ( $M^+ = Li^+, Na^+, K^+$ ) complexes: A quantum chemical study". **Chemical Physics**, 382, 5-14.
24. **Nidhi Vyas**, Animesh K. Ojha, (2010) "Interaction of alanine with small water clusters;  $Ala-(H_2O)_n$  ( $n = 1, 2$  and  $3$ ): A density functional study." **Journal of Molecular Structure: THEOCHEM** 940, 95-102.

#### ➤ Awards and Achievements

1. DST- INSPIRE Faculty Fellowship - 2016
2. DST-FAST TRACK for Young Scientist - 2012
3. Post Doctoral Fellowship, University of Calabria, Italy -2012
4. Best Poster Presentation Award, (National conference-2009 at CMP Degree College, University of Allahabad)
5. Senior Research Fellowship (SRF), MNNIT, Allahabad- April 2011-July 2009
6. Junior Research Fellowship (JRF), MNNIT, Allahabad- July 2009-July 2007
7. Graduate Aptitude Test in Engineering (GATE)-2007, 92. 00, Percentile \_

#### ➤ Workshops/Seminars/FDPs

##### Invited Talk

1. *Mechanistic Insights on the Oxygen Transfer Reactions of Manganese (III/IV)-Oxo Complexes: A DFT exploration: International Workshop on Modeling of Materials using CRYSTAL (IWMMS 2014)*, organized by Dept. of Physics Bundelkhand University, Jhansi, India in collaboration with Università di Torino, Torino, Italy and Michigan Technological University, Houghton, USA .
2. *DFT Studies on the Dinitrogen reduction into ammonia by iron-dinitrogen complexes bearing tripodal ligand: New Frontiers in Chemical Science (NFCS)*, organized by Department of Chemistry, IIT Bombay, and Mumbai, during 13<sup>th</sup> - 14<sup>th</sup> December, 2018.

##### Research Work Presented in International Conferences

1. **Vyas, N.**, Ansari, A.; Rajaraman, G. (2013) "Mechanistic Insight of the Oxygen Atom Transfer Reaction from  $Mn^{IV}$ -oxo Complex: DFT Exploration" Symposium on Modern Trends in Inorganic Chemistry – XV (MTIC-XV), December 13-16 IIT-Roorkee, India.
2. **Vyas, N.**; Raju, A.; Jaccob, M.; Rajaraman, G.(2013) "Generation of the Manganese (III/IV)-Oxo Complexes by Dioxygen Activation: A DFT Exploration" 3rd INDO-GERMAN conference on Modeling Chemical and Biochemical Reactivity. Febuary 26,- March 1. NIPER and IISER, Mohali, India
3. **Vyas, N.**; Ojha. A. K. (2010) "DFT study of cation  $(Mg)^{+2} - \pi$  interaction with different conformers of phenylalanine" International Conference on Perspectives in Vibrational Spectroscopy, February, 21-24, Banaras Hindu University, Varanasi, India.
4. **Vyas, N.**; Ojha. A. K. (2010) "Quantum chemical calculation of dissociation constant of some biologically important molecules" International Conference and Humboldt-Kollege on Frontiers of Environmental & Health Sciences Useful to Mankind: A Multidisciplinary Approach, February,24-27, University of Lucknow, Lucknow, India.

5. **Vyas, N.;** Ojha. A. K. (2008), "DFT study of many body interaction in alanine- (Water)<sub>1,2</sub> complex" International Conference and Humboldt-Kollege on Structural Characterization of Materials Relevant to Nanotechnology, Biomedical and Geobiology. November, 7-9 Banaras Hindu University, Varanasi, India.

#### National Conferences Attended

1. **Vyas, N.** (2014) 16<sup>th</sup> CRSI National Symposium in Chemistry (NSC-16) February 7-9, IIT Bombay, India.

#### Research Work Presented in National Conferences

1. **Vyas, N.;** Raju, A.; Jaccob, M.; Rajaraman, G. (2013) "Mechanistic Consideration of the Generation of Manganese (III/IV)-Oxo Complexes by Dioxygen Activation" Symposium on Theoretical and Computational Chemistry -Frontiers and Challenges. June, 14-15, Bharathidasan University, Tiruchirappalli.
2. **Vyas, N.;** Raju, A.; Jaccob, M.; Rajaraman, G. (2012) "Mechanistic insights of the manganese (III/IV)-oxo complexes: A DFT exploration" Theoretical Chemistry Symposium, December 19-22, IIT- Guwahati, India.
3. **Vyas, N.;** Raju, A.; Jaccob, M.; Rajaraman, G. (2012) "Generation and reactivity of Mn(III/IV)=O species: A theoretical exploration" Symposium on New Directions in Chemical Sciences, December 7-9, IIT-Delhi, India.
4. **Vyas, N.;** Ojha. A. K. (2010) "Combined effect of metal cations (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>) and water molecules on gas phase structural stability of neutral and zwitterionic alanine : A quantum chemical study" Theoretical Chemistry Symposium, December 8-12, IIT- Kanpur, India.
5. **Vyas, N.;** Ojha. A. K. (2009) "Calculation of dissociation constant and chemical hardness of biologically important molecules" National Conference on Application of Material Science In the Service of Society. CMP Degree College, September, 12-13, University of Allahabad, Allahabad, India (**Best Poster Award**).
6. **Vyas, N.;** Ojha. A. K. (2009) "DFT study of different conformers of glycine+(W)<sub>3</sub> complexes in different polar medium". Meghnad Saha Memorial Symposium on Emerging Trends in Laser & Spectroscopy and Application. March, 23-25. University of Allahabad. Allahabad, India.

#### School/Workshop Attended

1. **DST-SERC School in Atomic and Molecular Sciences**, 15 April - 5 May 2009, held at Physical Research Laboratory, Ahmadabad.
2. **Introduction to Gaussian: Theory and Practice**, 16-20 January, 2017, held at Radisson Blue Dwarka, New Delhi organized by Scube Scientific Software Solutions Pvt. Ltd.
3. **Workshop and Symposium on Advanced Simulation Methods: DFT, MD and Beyond**, March 6-10 2019 at Indian Institute of Technology Delhi, New Delhi, India, Jointly organized by Departments of Physics, Chemistry, Chemical Engineering, Civil Engineering, Materials Science and Engineering, Computer Services Centre, and the HPC Group.
4. **Workshop on in silico Quantum Modelling Studies** organized by Inter-University Accelerator Centre (IUAC), New Delhi., during 25-29 November 2019.

#### ➤ **Work experience:**

8 Years in R & D

#### **DST INSPIRE Faculty Fellowship, J.N.U. New Delhi**

Title of Project : Computational Exploration on the Reaction Mechanism of the Nitrogenase Enzyme using Density Functional Study

Cost of the Project : 35,00,000 (India Rupees- Thirty Five Lakh)

Funding Agency : Department of Science and Technology (DST), New Delhi, India.

Host Institute : School of Biotechnology, Jawaharlal Nehru University New Delhi.

Duration : April 2016-2022

**DST-FAST TRACK for Young Scientist Fellowship, IITB, Mumbai**

Title of Project :Computational exploration on the reaction mechanism of Fe mediated catalytic reactions: Emphasis to Methane Monoxygenase and extradiol catecholic dioxygenase enzymes

Cost of the Project : 27,00,000 (India Rupees- Twenty Seven Lakh)

Funding Agency : Department of Science and Technology (DST), New Delhi,India.