

Curriculum Vitae

Neha Agnihotri

Assistant Professor

Department of Physics

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Research Interests

- Graphene and other 2D Materials
- Design and Simulation of advanced functional materials
- Density Functional Theory

Academic Credentials

- **Assistant Professor (2018-present):** Department of Physics, NIT, Jamshedpur, India
- **DST-INSPIRE Faculty (2014-2018):** Department of Physics, IIT(BHU), Varanasi, India
- **Post Doctoral Fellow/Visiting Scholar (2012-2014):** University of Saskatchewan, Canada
- **Ph.D. (2011):** Physics, Banaras Hindu University, Varanasi, India

Awards and Recognitions

- DST-INSPIRE Faculty Award by DST, India
- Post Doctoral Fellowship awarded by University of Saskatchewan, Canada
- CSIR-National Eligibility Test (NET)
- Best paper presentation award in International conference on perspectives in vibrational spectroscopy (ICOPVS-2010) held at Banaras Hindu University, Varanasi, India
- Senior Research Fellowship awarded by CSIR, India
- UGC-Research Fellowship in Science for Meritorious Students (RFSMS) awarded by UGC, India

Sponsored Research Project

- **Project Title:** *Computational Modelling of Novel Materials for Efficient, Robust Organic Solar Photovoltaic Cells*; funded by Department of Science & Technology, New Delhi, India, 2014-2020 (35.0 Lakhs)

Facility Established

- Dell Cluster for High performance computing (HPC).
- 03 Desktop computers for simulation
- Gaussian Code for First Principles Calculations

Research Publications

- Vinita, M. Tiwari, **Neha Agnihotri**, M. Singh, A. K. Singh, R. Prakash, (2019) *Nanonetwork of Coordination Polymer AHMT-Ag for the Effective and Broad Spectrum Detection of 6-Mercaptopurine in Urine and Blood Serum* **ACS Omega** 4, 16733.
- **Neha Agnihotri***, (2019) *Strong, near-infrared absorbing porphyrins: a DFT study* **Can. J. Chem.** 97, 451.
- **Neha Agnihotri***, (2016) *Computational Modelling of Panchromatic Porphyrins with Strong NIR Absorptions for Solar Energy Capture*, **Chem. Phys. Lett.** 665, 40. (**Editor's choice article**)
- **Neha Agnihotri***, R. P. Steer, (2016) *Time Dependent DFT Investigation of the Optical Properties of Artificial Light Harvesting Special Pairs*, **Phys. Chem. Chem. Phys.** 18, 15337.
- **Neha Agnihotri**, R. P. Steer, (2015) *DFT and TD-DFT calculations of axially substituted tin porphyrins and an ethynyl-linked tin porphyrin dimer*, **J. Porphyrins Phthalocyanines** 19, 610.
- **Neha Agnihotri**, R. P. Steer, (2014) *TD-DFT calculations of the excited states of metalloporphyrins relevant to organic solar photovoltaic cells*, **J. Porphyrins Phthalocyanines** 18, 475.
- **Neha Agnihotri***, (2014) *Computational studies of charge transfer in organic solar photovoltaic cells: a Review*, **J. Photochem. Photobiol. C: Photochemistry Reviews** 18, 18. (**I.F.:10.4**)
- **Neha Agnihotri**, P.C. Mishra (2011) *Scavenging mechanism of curcumin towards the hydroxyl radical: A theoretical study of reactions producing ferulic acid and vanillin*, **J. Phys. Chem. A** 115, 14221.
- **Neha Agnihotri**, P.C. Mishra (2011) *Hybridization-displaced charges for amino-acids: a new model using two point charges per atom along with bond-center charges*, **J. Mol. Model.** 17, 1435.
- Saumya Tiwari, **Neha Agnihotri**, P. C. Mishra (2011) *Quantum Theoretical Study of Cleavage of the Glycosidic Bond of 2'-Deoxyadenosine: Base Excision-Repair Mechanism of DNA by MutY*, **J. Phys. Chem. B** 115, 3200.
- **Neha Agnihotri**, P.C.Mishra (2011) *Reactivities of radicals of adenine and guanine towards reactive oxygen species and reactive nitrogen oxide species: OH[•] and NO₂[•]*, **Chem. Phys. Lett.** 503, 305.
- **Neha Agnihotri**, P.C. Mishra (2010) *Formation of 8-Nitroguanine due to reaction between guanyl radical and nitrogen dioxide: Catalytic role of hydration*, **J. Phys. Chem. B** 114, 7391.
- **Neha Agnihotri**, P.C. Mishra (2009) *Mechanism of scavenging action of N-acetylcysteine for the OH radical: A quantum computational study*, **J. Phys. Chem. B** 113, 12096.

- **Neha Agnihotri**, P.C. Mishra (2009) *Mutagenic product formation due to reaction of guanine radical cation with nitrogen dioxide*, **J. Phys. Chem. B** 113, 3129.

Book Chapter

- N. R. Jena, **Neha Agnihotri**, P. C. Mishra, (2014) *Formation of DNA Lesions, its Prevention and Repair* in the Book Titled: Application of Computational Techniques in Pharmacy and Medicine (*Springer*) ISBN: 978-94-017-9256-1

Conferences/Short Term Courses

- **Invited Talk:** *Electronic properties of graphene nanoribbons* at Symposium on Carbon Nanomaterial Electronics-2019 (SCNE-2019), Birla Institute of Science and Technology (BITS), Pilani, India (November 08, 2019).
- AICTE Sponsored QIP-Short Term Course on *Radiation Effects in Materials and Their Characterizations through Advanced Techniques* at Indian Institute of Technology (IIT-BHU) Varanasi, India (October 07-11, 2019).
- *First-Principles Modelling of Dye Sensitized Solar Cells under "Young Scientist Award Category"* at International Conference on Functional Nano-Materials (ICFNM-2019), Indian Institute of Technology (IIT-BHU), Varanasi, India (February 24, 2019).
- *Computational Modelling of Panchromatic Porphyrins for Solar Photovoltaic Cells* at 2nd Meghnad Saha Memorial International Symposium-cum-Workshop on Laser Induced Breakdown Spectroscopy, (MMISLIBS-II 2018), University of Allahabad, Allahabad, India (February 19, 2018).
- **Invited Talk:** *Panchromatic Absorbers for Harvesting Solar Energy* at International Conference on Nanotechnology: Ideas, Innovations and Initiatives-2017 (ICN:3I-2017), Indian Institute of Technology (IIT) Roorkee, India (December 08, 2017).
- *Computational Modelling of Novel Materials for Light Harvesting* at International Workshop & Conference on Frontiers of Spectroscopy, Banaras Hindu University, Varanasi, India (January 12, 2015).
- *Curcumin: A potent antioxidant for OH radical* at 2nd International Workshop on Spectroscopic Signatures of Molecular Complexes/Ions in our Atmosphere and Beyond, Banaras Hindu University, Varanasi, India (February 08, 2012).
- *Base-excision repair mechanism of DNA by enzyme MutY: A quantum computational study* at 7th Asian Biophysics Association (ABA) symposium & Annual meeting of the Indian biophysical society (IBS) All India Institute of Medical Sciences (AIIMS), New Delhi, India (January 30, 2011).
- *A quantum computational approach to study Base-excision repair mechanism of DNA* at Meghnad Saha Memorial International Symposium-cum-workshop on Laser-induced breakdown spectroscopy (MMISLIBS), University of Allahabad, Allahabad, India (December 22, 2010).

- *A quantum mechanical approach to study DNA damage and its consequence at the molecular level at 98th Indian Science Congress under “ISCA Young Scientists Award Programme” in the Section of Physical Sciences, SRM University, Chennai, India (October 03, 2010).*
- *Mechanism of antioxidant action of N-Acetylcysteine for the hydroxyl radical: A quantum computational study at 3rd One Day Conference on New Trends in Research, Banaras Hindu University, Varanasi, India (March 30, 2010).*
- *A quantum computational study of the hydroxyl radical scavenging ability of N-Acetylcysteine at International Conference and Humboldt Kolleg, University of Lucknow, Lucknow, India (February 25, 2010).*
- *Reaction of guanine radical cation with nitrogen dioxide: A quantum computational study at International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS), Banaras Hindu University, Varanasi, India (February 22, 2010).*
- *A quantum computational study for the formation of mutagenic product 8-nitroguanine⁺ at Symposium on Recent Trends in Biophysics and Workshop on Emerging Techniques of Biophysics, Banaras Hindu University, Varanasi, India (February 14, 2010).*
- *A density functional theoretic study of reaction of guanine radical cation with nitrogen dioxide radical at 2nd One Day Conference on New Trends in Research, Banaras Hindu University, Varanasi, India (January 17, 2009).*

Professional Memberships

- Life Member of the Laser and Spectroscopic Society of India (LASSI).
- Life Member of the Indian Science Congress Association (ISCA).

Reviewer Experience

Reviewed manuscripts for:

- Physical Chemistry Chemical Physics (Royal Society of Chemistry)
- Journal of Physical Chemistry (American Chemical Society)
- Journal of Chemical Physics (American Institute of Physics)
- Chemical Physics (Elsevier)
- Journal of Molecular Graphics and Modelling (Elsevier)

Teaching

- Thermodynamics and Statistical Mechanics (NIT-JSR)
- Computational Physics (NIT-JSR)
- Nuclear Physics (NIT-JSR)
- Particle Physics (NIT-JSR)
- Modern Physics (IIT-BHU)
- Classical, Quantum & Relativistic Mechanics (IIT-BHU)
- Introduction to Renewable Energy Sources (IIT-BHU)

- Nuclear & Particle Physics (IIT-BHU)
- Classical and Quantum Physics (IIT-BHU)

Supervision

- Ph. D. Thesis (**01 ongoing**)
 - Master's Thesis (**06 completed**)
 - Undergraduate projects (**05 completed**)
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