

## Curriculum Vitae

**Dr. P. K. Shukla**  
Associate Professor

**Department of Physics, Assam University, Silchar**

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**VIDWAN PROFILE:**

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**Google Scholar:**

<https://scholar.google.com/citations?user=bIvcZdUAAAAJ&hl=en&authuser=3>

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### **1. Educational Background**

| Examination      | Board/University                   | Marks  | Year |
|------------------|------------------------------------|--------|------|
| Ph. D. (Physics) | Banaras Hindu University, Varanasi | N.A.   | 2008 |
| M. Sc. (Physics) | VBS Purvanchal University, Jaunpur | 75.4 % | 2002 |
| B. Sc.           | VBS Purvanchal University, Jaunpur | 67.3 % | 2000 |
| Intermediate     | U.P. Board Allahabad               | 70.8 % | 1997 |
| High School      | U.P. Board Allahabad               | 76.3 % | 1995 |

Ph. D. Thesis Title - *Study of Electronic Structure, Properties, Interactions and Reactions of Some Biologically Important Molecules and Other Molecules*

Ph. D. Supervisor: Late Prof. P.C. Mishra, Physics Deptt., B.H.U., Varanasi.

### **2. Research Interests**

- ◆ Quantum Mechanical Ab-Initio and Density Functional Theory (DFT) Calculations
- ◆ Molecular Modeling
- ◆ Carbon nanomaterials (CNTs and graphene-based materials)
- ◆ Photovoltaic materials
- ◆ Biomolecular interactions and reactions
- ◆ Design and properties of metal-based anticancer drugs
- ◆ DNA Damage & Repair
- ◆ Unnatural nucleobases
- ◆ Antioxidants
- ◆ Solvent effects (Bulk and Specific), etc.

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### **3. Work Experience**

- March 2022 – Present** Associate Professor, Department of Physics, Assam University, Silchar, Assam, **Teaching & Research.**
- March 2010 – March 2022** Assistant Professor (Stage I, II & III), Department of Physics, Assam University, Silchar, Assam, **Teaching & Research.**
- Aug. 2013 – July 2014** Visiting Scientist, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, U.S.A. **Research**, Advisor: **Professor Jean-Luc Bredas.** (On study leave from Assam University)
- Nov. 2008 – March 2010** Senior Research Fellow (SRF), Department of Physics, B.H.U., Varanasi, in a CSIR sponsored research project under Prof. P.C. Mishra. **Research**
- Oct. 2005 – Nov. 2008** JRF & SRF (through CSIR-UGC Joint Test), Department of Physics, B.H.U., Varanasi. **Research**

### **4. Awards/Fellowships**

- ◆ INSA Visiting Scientist Award for visiting Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru. **Award Year: 2019**
- ◆ UGC Raman Fellowship for Post Doctoral Studies in USA under Indo-US 21<sup>st</sup> Century Knowledge Initiative for a period of one Year. **Award Year: 2013**
- ◆ DST Young Scientist Travel Grant for participating in 13-ICQC held at the **University of Helsinki, Helsinki (Finland)** during June 22-27, **2009.**
- ◆ Offer of Post Doctoral Position from University of South Florida, Tampa, U.S.A., **2010.**
- ◆ Best Oral Presentation Award in “*1<sup>st</sup> One Day Conference on New Trends in Research*” held at the Department of Physics, Banaras Hindu University, Varanasi, on Oct. 27, **2007.**
- ◆ Qualified **NET-JRF** in *Physical Sciences Section* conducted by CSIR-UGC, New Delhi jointly, **Dec. 2004.**
- ◆ Qualified Uttar Pradesh State Level Eligibility Test (**UP-SLET**) in *Physical Sciences*, **2004.**
- ◆ National Scholarship in Intermediate [**1995-1997**]

### **5. Research Projects (Completed/Ongoing)**

| <b>Project Title</b>  | <b>Funding Agency</b> | <b>Duration</b> | <b>Amount (Lakhs)</b> |
|---|-----------------------|-----------------|-----------------------|
| Molecular Mechanisms of Action of Ruthenium Anticancer Drugs: A Quantum Computational Study | S.E.R.B., New Delhi   | 2015-2018       | 19.39                 |
|   |                       |                 |                       |

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### 6. Research Guidance

| Research Supervision | Ph. D.         |                  |         | M. Phil. Awarded | P.G. Degree Awarded |
|----------------------|----------------|------------------|---------|------------------|---------------------|
|                      | Degree Awarded | Thesis Submitted | Ongoing |                  |                     |
| Sole Supervisor      | 3              | 0                | 3       | 01               | 44                  |
|                      |                |                  |         |                  |                     |

### 7. List of Publications (\* denotes corresponding author); h-index: 14

#### (A) Journal Articles:

43. B. I. Laskar and **P. K. Shukla\***

Potential of graphene as an adsorbent for HSSS· Radical – A DFT study, *Physica B: Condensed Matter* **2024** (Published Online).

DOI: <https://doi.org/10.1016/j.physb.2024.416428>

42. S. Biswas and **P. K. Shukla\***

Reactions of chlorophyll with hydroxyl radicals via RAF, HAT and SET mechanisms: A theoretical study, *Structural Chemistry* **2024** (Published Online).

DOI: <https://doi.org/10.1007/s11224-024-02331-3>

41. N. R. Jena and **P. K. Shukla**

Hydroxyl radical-induced C1'-H Abstraction Reaction of Different Artificial Nucleotides, *Journal of Molecular Modeling* **2024**, 30, 330.

DOI: <https://doi.org/10.1007/s00894-024-06126-5>

40. N. R. Jena and **P. K. Shukla**

Structure and stability of different triplets involving artificial nucleobases: clues for the formation of semisynthetic triple helical DNA, *Scientific Reports* **2023**, 13, 19246.

DOI: <https://doi.org/10.1038/s41598-023-46572-4>

39. B. I. Laskar, A. K. Mishra and **P. K. Shukla\***

Role of graphene in scavenging methyl cations: A DFT study, *Journal of Molecular Modeling* **2023**, 29, 299.

DOI: <https://doi.org/10.1007/s00894-023-05662-w>

38. B. I. Laskar and **P. K. Shukla\***

Methylation of graphene (pristine and S-doped) by carcinogenic methane diazonium ion: A DFT Study, *Molecular Simulation* **2023**, 49, 1512-1518.

DOI: <https://doi.org/10.1080/08927022.2023.2245070>

37. D. Khiangte, B. Hazarika, S. Biswas, Lalhrui, R. Kataria, **P. K. Shukla**, V. P. Singh

## Curriculum Vitae

Design, synthesis and structural study of two symmetry-independent pyridone analogue in the asymmetric unit, *Journal of Molecular Structure* **2023**, 1291, 135856.

DOI: <https://doi.org/10.1016/j.molstruc.2023.135856>

36. N. R. Jena, P. Das and **P. K. Shukla**

Complementary base pair interactions between different rare tautomers of the second-generation artificial genetic alphabets, *Journal of Molecular Modeling* **2023**, 29, 125 (11 pages).

DOI: <https://doi.org/10.1007/s00894-023-05537-0>

35. S. Biswas and **P. K. Shukla\***

A DFT study on the scavenging activity of curcumin toward methyl and ethyl radicals, *Molecular Simulation*, **2023**, 49, 589-598.

DOI: <https://doi.org/10.1080/08927022.2023.2178236>

34. P. K. Shah, N. R. Jena and **P. K. Shukla\***

A theoretical characterization of mechanisms of action of osmium(III)-based drug Os-KP418: hydrolysis and its binding with guanine, *Structural Chemistry* **2023**, 34, 995–1003.

DOI: <https://doi.org/10.1007/s11224-022-02064-1>

33. P. K. Shah, N. R. Jena and **P. K. Shukla\***

Reactions of Ru(III)-drugs KP1019 and KP418 with guanine, 2'-deoxyguanosine and guanosine: a DFT study, *Journal of Molecular Modeling* **2022**, 28, 291 (8 pages).

DOI: <https://doi.org/10.1007/s00894-022-05304-7>

32. J. Dowarah, B. N. Marak, B. S. Sran, P. K. Shah, **P. K. Shukla** and V. P. Singh

Synthesis of a pyridone-based phthalimide fleximer and its characterization and supramolecular property evaluation, *ACS Omega* **2022**, 7, 24485–24497.

DOI: <https://doi.org/10.1021/acsomega.2c02095>

31. P. K. Shah and **P. K. Shukla\***

Formation of bifunctional cross-linked products due to reaction of NAMI-A with DNA bases – A DFT Study, *Structural Chemistry* **2022**, 33, 807-814.

DOI: <https://doi.org/10.1007/s11224-022-01897-0>

30. S. Biswas and **P. K. Shukla\***

Effect of N7-methylation on base pairing patterns of guanine: a DFT study, *Journal of Molecular Modeling* **2021**, 27, 184 (9 pages).

DOI: <https://doi.org/10.1007/s00894-021-04792-3>

29. B. I. Laskar and **P. K. Shukla\***

Adsorption of HOOO· radical on pristine and doped graphene – A first-principles study, *Structural Chemistry* **2021**, 32, 1171-1179.

DOI: <https://doi.org/10.1007/s11224-020-01702-w>

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28. J. Dowarah, D. Patel, B. N. Marak, U.C.S. Yadav, P.K. Shah, **P.K. Shukla** and V.P. Singh  
Green synthesis, structural analysis and anticancer activity of dihydropyrimidinones derivatives, *RSC Advances* **2021**, 11, 35737-35753.  
DOI: <https://doi.org/10.1039/D1RA03969E>
27. Z. H. Mazumder, D. Sharma, D. Sengupta, A. Mukherjee, J. S. Boruah, S. Basu, **P. K. Shukla**, T. Jha  
Photodynamic activity attained through raptured  $\pi$ -conjugation of pyridyl groups with a porphyrin macrocycle: Synthesis, Photophysical and Photobiological Evaluation of 5-mono-(4-nitrophenyl)-10,15,20-tris-[4-(phenoxyethyl)pyridine] porphyrin and its Zn(II) complex, *Photochemical & Photobiological Sciences* **2020**, 19, 1776-1789.  
DOI: <https://doi.org/10.1039/D0PP00319K>
26. Z. H. Mazumder, D. Sharma, A. Mukherjee, S. Basu, **P. K. Shukla**, T. Jha, D. Sengupta  
meso-Thiophenium Porphyrins and Their Zn(II) Complexes: A New Category of Cationic Photosensitizers, *ACS Medicinal Chemistry Letters* **2020**, 11, 2041-2047.  
DOI: <https://doi.org/10.1021/acsmchemlett.0c00266>
25. P. K. Shah and **P. K. Shukla\***  
A DFT Study of Reactions of Ru(III) Anticancer Drug KP1019 with 8-Oxoguanine and 8-Oxoadenine, *Structural Chemistry* **2020**, 31, 2087-2092.  
DOI: <https://doi.org/10.1007/s11224-020-01563-3>
24. P. K. Shah and **P. K. Shukla\***  
Effect of Axial Ligands on the Mechanisms of Action of Ru(III) Complexes Structurally Similar to NAMI-A: A DFT study, *Structural Chemistry* **2020**, 31, 679-689.  
DOI: <https://doi.org/10.1007/s11224-019-01439-1>
23. S. Biswas, P. K. Shah and **P. K. Shukla\***  
Methylation of DNA Bases by Methyl Free Radicals: Mechanism of Formation of C8-Methylguanine, *Structural Chemistry* **2018**, 29, 1333-1340.  
DOI: <https://doi.org/10.1007/s11224-018-1118-0>
22. K. Bhattacharjee and **P. K. Shukla\***  
A Theoretical Characterization of Reactions of HOOO Radical with Guanine: Formation of 8-Oxoguanine, *Structural Chemistry* **2018**, 29, 1109-1118.  
DOI: <https://doi.org/10.1007/s11224-018-1095-3>
21. K. Bhattacharjee and **P. K. Shukla\***  
Does 8-Nitroguanine Form 8-Oxoguanine? An Insight from Its Reaction with  $\bullet$ OH Radical, *Journal of Physical Chemistry B* **2018**, 122, 1852-1861.  
DOI: <https://doi.org/10.1021/acs.jpcc.7b12192>
20. K. Bhattacharjee, P. C. Mishra and **P. K. Shukla\***

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Mechanism of Methylation of 8-Oxoguanine due to Its Reaction with Methyl Diazonium Ion, *Molecular Simulation* **2017**, 43, 196-204.

DOI: <https://doi.org/10.1080/08927022.2016.1246734>

19. P. K. Shah, K. Bhattacharjee and **P. K. Shukla\***

Mechanisms of Reactions of Ru(III)-Based Drug NAMI-A and Its Aquated Products with DNA Purine Bases: A DFT Study, *RSC Advances* **2016**, 6, 113620-113629.

DOI: <https://doi.org/10.1039/C6RA24251K>

18. K. Bhattacharjee and **P. K. Shukla\***

A DFT Study of Reactions of Methyl Diazonium Ion with DNA/RNA Nucleosides: Investigating Effect of Sugar Moiety on Methylation Pattern of Bases, *International Journal of Quantum Chemistry* **2014**, 114, 1637-1644.

DOI: <https://doi.org/10.1002/qua.24733>

17. J. Warnan, A. El Labban, C. Cabanetos, E. T. Hoke, **P. K. Shukla**, C. Risko, J.- L. Brédas, M. D. McGehee and P. M. Beaujuge

Ring Substituents Mediate the Morphology of PBDTTPD-PCBM Bulk-Heterojunction Solar Cells, *Chemistry of Materials* **2014**, 26, 2299-2306.

DOI: <https://doi.org/10.1021/cm500172w>

16. **P. K. Shukla\*** and P. C. Mishra

Base Pairing Patterns of DNA Base Lesion Spiroiminodihydantoin: A DFT Study, *International Journal of Quantum Chemistry* **2013**, 113, 2600-2604.

DOI: <https://doi.org/10.1002/qua.24512>

15. **P. K. Shukla**, Vinay Ganapathy and P. C. Mishra

A Quantum Theoretical Study of Reactions of Methyl Diazonium Ion With DNA Base Pairs, *Chemical Physics* **2011**, 388, 31-37.

DOI: <https://doi.org/10.1016/j.chemphys.2011.07.014>

14. **P. K. Shukla**, N. R. Jena and P. C. Mishra

Quantum Theoretical Study of Molecular Mechanisms of Mutation and Cancer: A Review, *Proc. Natl. Acad. Sc., India, Section A- Physical Sciences*, **2011**, 81A, 79-98.

Link: <http://eprints.iisc.ac.in/id/eprint/39081>

13. **P. K. Shukla**, N. Kumar and P. C. Mishra

Hydrogen Atom Abstractions of the Sugar Moiety of 2'-Deoxyguanosine with an OH Radical: A Quantum Chemical Study, *International Journal of Quantum Chemistry* **2011**, 111, 2160-2169.

DOI: <https://doi.org/10.1002/qua.22494>

12. N. Kumar, **P. K. Shukla** and P. C. Mishra

Reactions of the OOH radical With Guanine: Mechanisms of Formation of 8-Oxoguanine and Other Products, *Chemical Physics* **2010**, 375, 118-129.

DOI: <https://doi.org/10.1016/j.chemphys.2010.08.004>

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11. **P. K. Shukla** and P. C. Mishra  
Effects of Diameter, Length, Chirality and Defects on the Scavenging Action of Single-Walled Carbon Nanotubes for OH Radicals: A Quantum Computational Study, *Chemical Physics* **2010**, 369, 101-107.  
DOI: <https://doi.org/10.1016/j.chemphys.2010.03.011>
10. N. Dixit, **P. K. Shukla**, P. C. Mishra, L. Mishra and H.W. Roesky  
Binding of Urea and Thiourea with a Barbiturate Derivative: Experimental and Theoretical Approach, *Journal of Physical Chemistry A* **2010**, 114, 97-104.  
DOI: <https://doi.org/10.1021/jp906909y>
9. **P. K. Shukla** and P. C. Mishra  
A Quantum Chemical Study of Reactions of DNA Bases with Sulphur Mustard: A Chemical Warfare Agent, *Theoretical Chemistry Accounts* **2010**, 125, 269-278.  
DOI: <https://doi.org/10.1007/s00214-009-0514-3>
8. N. R. Jena, **P. K. Shukla**, H. S. Jena, P. C. Mishra and S. Suhai  
O6-Methylguanine Repair by O6-Alkylguanine-DNA Alkyltransferase, *Journal of Physical Chemistry B* **2009**, 113, 16285-16290.  
DOI: <https://doi.org/10.1021/jp907836w>
7. **P. K. Shukla** and P. C. Mishra  
Repair of O6-Methylguanine to Guanine by Cysteine in the Absence and Presence of Histidine and by Cysteine Thiolate Anion: A Quantum Chemical Study, *Physical Chemistry Chemical Physics* **2009**, 11, 8191-8202.  
DOI: <https://doi.org/10.1039/B908295F>
6. S. Tiwari, **P. K. Shukla** and P. C. Mishra  
Improved Electrostatic Properties Using Combined Mulliken and Hybridization- Displaced Charges for Radicals, *Journal of Molecular Modeling* **2008**, 14, 631-640.  
DOI: <https://doi.org/10.1007/s00894-008-0308-x>
5. **P. K. Shukla** and P. C. Mishra  
Reactions of NO<sub>2</sub>Cl with Imidazole: A Model Study for the Corresponding Reactions of Guanine, *Journal of Physical Chemistry B* **2008**, 112, 7925-7936.  
DOI: <https://doi.org/10.1021/jp801093r>
4. **P. K. Shukla** and P. C. Mishra  
Catalytic Involvement of CO<sub>2</sub> in the Mutagenesis Caused by Reactions of ONOO<sup>-</sup> With Guanine, *Journal of Physical Chemistry B* **2008**, 112, 4779-4789.  
DOI: <https://doi.org/10.1021/jp710418b>
3. **P. K. Shukla**, P. C. Mishra and S. Suhai  
Reactions of DNA Bases with the Anti-Cancer Nitrogen Mustard Mechlorethamine: A Quantum Chemical Study, *Chemical Physics Letters* **2007**, 449, 323-328.

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DOI: <https://doi.org/10.1016/j.cplett.2007.10.072>

2. **P. K. Shukla** and P. C. Mishra

H<sub>2</sub>O<sub>3</sub> as a Reactive Oxygen Species: Formation of 8-Oxoguanine from Its Reaction with Guanine, *Journal of Physical Chemistry B* **2007**, 111, 4603-4615.

DOI: <https://doi.org/10.1021/jp070399e>

1. **P. K. Shukla**, P. C. Mishra and S. Suhai

Reactions of Guanine with Methyl Chloride and Methyl Bromide: O6-Methylation Versus Charge Transfer Complex Formation, *International Journal of Quantum Chemistry* **2007**, 107, 1270-1283.

DOI: <https://doi.org/10.1002/qua.21233>

### **(B) Book Chapters**

1. **P. K. Shukla** and P. C. Mishra

DNA Lesions Caused by ROS and RNOS: A Review of Interactions and Reactions Involving Guanine, in Practical Aspects of Computational Chemistry. J. Leszczynski and M. K. Shukla (Eds), Springer, 2010, DOI: 10.1007/978-90-481-2687-3\_22. ISBN: 978-90-481-2686-6

### **8. Invited Talks:**

11. Talk titled “Density functional theory and its applications: Some examples” in Topical Research School on Recent Trends of Research in Theoretical and Experimental Physics organized by the Department of Physics, Gurucharan College, Silchar, during March 11-13, 2024.
10. Talk titled “Investigating role of graphene in scavenging some DNA damaging agents: A DFT approach” in the 3<sup>rd</sup> International Conference on Advancement in Core and Frontier of Physics (ACFP-2024) organized by the Department of Physics, GLA University, Mathura, during February 2-4, 2024.
9. Talk titled “Graphene as a scavenger of carcinogenic methylating agents: A DFT exploration” in the International Conference on Advances in Spectroscopic Techniques and Materials (ASTM-2024) organized by the Department of Physics, IIT (ISM) Dhanbad, during January 18-20, 2024.
8. Lecture titled “Application of density functional theory in drug design” in the DBT-Sponsored workshop on “Computational Approaches in Drug Designing: 2.0” organized by the Bioinformatics & Computational Biology Centre, Assam University, Silchar, during December 13-19, 2023.
7. Talk titled “Role of density functional theory in science and technology” in the Special Summer School on Emerging Trends in Science and Technology organized by the UGC-HRDC, Mizoram University, Aizawl, during August 3-16, 2023.
6. Talk titled “Insight into the interactions of Ru(III)-anticancer drugs with DNA from a DFT perspective” in the International Conference on Science and Technology for Innovative and Sustainable Development (STISD-2023) organized by the Department of Chemistry and Industrial Chemistry, Mizoram University, Aizawl, during June 28-30, 2023.



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5. Talk titled “Density functional theory: A versatile method for characterization of materials” in the Online one-week workshop on “Advanced Physical Tools and Techniques for Materials Characterization” (APTTMC-2020) organized by the Department of Physics, Mahatma Gandhi Central University, Motihari-845401, Bihar, during July 28 – August 03, 2020.
4. Talk titled “Understanding molecular mechanisms of action of ruthenium anticancer drugs using DFT calculations” at the National Conference on “Physics and Chemistry of Advanced Materials (NCPCAM-2019)” organized by the Department of Physics, Mahatma Gandhi Central University, Motihari-845401, Bihar, during November 22-23, 2019.
3. Talk titled “Molecular mechanisms of formation of mutagenic DNA lesions: A DFT study” at the 2<sup>nd</sup> National Conference on Hard and Soft Condensed Matter Physics (NCHSCMP-2019) held during March 4-6, 2019, at the Department of Physics, Tezpur University, Tezpur, Assam, India.
2. Talk titled “Molecular Mechanisms of Ruthenium Anticancer Drug – DNA Interaction” at the 6<sup>th</sup> International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2016) held during Nov. 5-8, 2016 organized by the University of Lucknow, Lucknow, India.
1. Talk titled “Quantum Chemical Modelling of PBDTTPD polymers for highly-efficient organic solar cells” at the National Symposium on Innovations in Product Design (IPD-2015) held during May 11-13, 2015, at the PDPM Indian Institute of Information Technology, Design and Manufacturing (IIITDM), Jabalpur, M.P., India

### **9. Participation in seminars/conferences etc.**

#### ***(A) International Seminars/Conferences***

8. **Participated** in the International e-conference on “Prospective of Interdisciplinary Research in Science and Technology in the Present Scenario”, organized by the Department of Physics, Chaudhary Charan Singh University, Meerut, U.P. on May 15-16, 2020.
7. **Paper Presentation (Oral)** entitled “Theoretical Study of DNA Damage at Molecular Level” in the XXVII IUPAP International Conference on Computational Physics (CCP2015) held during December 2-5, 2015, at the IIT Guwahati, Assam, India.
6. **Paper Presentation (Oral)** entitled “Effect of Ring Substituted Side Chains on the Electronic and Optical Properties of PBDTTPD Polymers: A Theoretical Study” in the International Conference on Frontiers of Spectroscopy (ICFS-2015) held during January 10-12, 2015, at the Department of Physics, Banaras Hindu University, Varanasi, U.P., India.
5. **Participated** in the Georgia Tech-COPE 10<sup>th</sup> Anniversary Symposium on March 14, 2014 at the Georgia Tech Global Learning Center, Atlanta, U.S.A.
4. **Participated** in the Theoretical Chemistry Day Symposium on October 15, 2013 at the School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, U.S.A.
3. **Paper Presentation (Poster)** entitled “Potential of Single-Walled Carbon Nanotubes as the Hydroxyl Radical Scavengers: A Quantum Chemical Approach” in the International Conference & Humboldt Kolleg on “Frontiers of Environmental & Health Sciences Useful to Mankind: A

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Multidisciplinary Approach” organized during February 24-27, 2010 by University of Lucknow and Humboldt Academy Lucknow at the University of Lucknow, U.P., India.

2. **Paper Presentation (Poster)** entitled “CO<sub>2</sub> as a Catalyst in the Formation of 8-Oxoguanine and 8-Nitroguanine Due to Reaction of ONOO<sup>-</sup> with Guanine: A DFT Study” in the 13<sup>th</sup> International Congress of Quantum Chemistry (13-ICQC) held during June 22-27, 2009, at the University of Helsinki, Helsinki, Finland.
1. **Paper Presentation (Poster)** entitled “Can H<sub>2</sub>O<sub>3</sub> Oxidize Guanine Forming Mutagenic Product 8-Oxoguanine More Efficiently Than H<sub>2</sub>O<sub>2</sub>? A Quantum Chemical Study” in the International Conference & Humboldt-Kolleg on “Structural Characterization and Spectroscopy on Materials Relevant to Nanotechnology, Biomedical and Geobiology” held during November 7-9, 2008, at Department of Physics, B.H.U., Varanasi, India.

### **(B) National Seminars/Conferences**

6. **Paper Presentation (Oral)** entitled “Understanding Molecular Mechanisms of Action of Os(III)-drugs Os-KP418 using DFT Calculations” in the XIII Biennial National Conference of Physics Academy of North East (PANE-2022) held during November 8-10, 2022, organized by the Department of Physics, Manipur University, Imphal.
5. **Paper Presentation (Poster)** entitled “Repair of O6-Methylguanine to Guanine by the Active Site Amino Acid Residues of O6-Alkylguanine-DNA Alkyltransferase” in the National Symposium on “Recent Trends in Biophysics” held during February 13-15, 2010, at the Department of Physics, Banaras Hindu University, Varanasi, U.P., India
4. **Paper Presentation (Oral)** entitled “Study of Electronic Structure, Properties, Interactions and Reactions of Some Biologically Important Molecules and Other Molecules” in the National Symposium on “Advances in Laser and Spectroscopic” held during February 27-28, 2009, at the Department of Physics, Dr. Hari Singh Gour University, Sagar, M.P., India
3. **Paper Presentation (Oral)** entitled “A Quantum Chemical Approach to the Understanding of Molecular Mechanisms of Mutation and Cancer” in the 96<sup>th</sup> Indian Science Congress under “*ISCA Young Scientists Award Programme*” in the Section of Physical Sciences, held on October 17, 2008, at the North Eastern Hill University, Shillong, Meghalaya, India.
2. **Paper Presentation (Oral)** entitled “A Quantum Chemical Approach to Oxidative Nature of H<sub>2</sub>O<sub>3</sub>: Formation of The Mutagenic Agent 8-Oxoguanine” in the *1<sup>st</sup> One Day Conference on New Trends in Research*” held on October 27, 2007, at the Department of Physics, Banaras Hindu University, Varanasi, U.P., India.
1. **Paper Presentation (Oral)** entitled “O6-Methylation of Guanine due to its Reaction with Methyl Chloride” in the National Symposium on Atomic, Molecular and Laser Physics (NSAMLP-2007) held during March 17-19, 2007, at Department of Physics, BHU, Varanasi, U.P., India.

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### **10. Participation in FDP/Workshops/etc.**

10. **Attended** the UGC-Sponsored Refresher Course in Physics (SRC) organized by the CPDHE (UGC-HRD), University of Delhi, Delhi, during October 4-18, 2021.
9. **Participated** in the FDP on Pedagogical Practices of New India under National Education Policy, 2020, organized jointly by the Assam University, Tripura University, and Manipur University, during October 7-11, 2020.
8. **Attended** Faculty Development Programme on “*Managing online classes and co-creating moocs: 2.0*” organized by Teachers Training Centre, Ramanujan College, University of Delhi, during May 18 – June 03, 2020.
7. **Attended** the UGC-Sponsored “*Refresher Course in Physics*” organized by the UGC-Human Resource Development Centre, University of Allahabad, Allahabad, during November 12-Dec. 02, 2018.
6. **Participated** in the Summer School 2017 on “*Electronic structure and spectroscopy of transition metal complexes*” organized by the Max Planck Institute of Chemical Energy Conversion, Germany at the Wissenschaftspark, Gelsenkirchen, Germany, during Sept. 03-09, 2017.
5. **Participated** in the Workshop on “*Statistical Physics of Soft Matter (SPSM-2015)*” organized by the Department of Physics, B.H.U., Varanasi, under UGC-Networking Programme, during November 26-30, 2015.
4. **Participated** in the “*Hands-on Workshop on Computational Biophysics*” organized by the National Center for Multiscale Modeling of Biological Systems (MMBioS) and the NIH Center for Macromolecular Modeling & Bioinformatics during May 19-23, 2014 in Pittsburgh, PA, U.S.A.
3. **Attended** the UGC-Sponsored “*Refresher Course in Physics*” organized by the Academic Staff College-Kurukshetra University at the Department of Physics, Kurukshetra Univ., Kurukshetra, Haryana, India, during May 02-22, 2103.
2. **Attended** the UGC-Sponsored “*59th Orientation Course*” organized by the Academic Staff College-B.H.U., Varanasi during January 03-30, 2012.
1. **Participated** in the winter school entitled, “*Winter School on Recent Trends in Physics of Atoms, Molecules and Lasers*” organized by the Department of Physics, Banaras Hindu University, Varanasi under the UGC Networking Program during January 09-31, 2011.

### **11. Contribution in organizing academic events:**

7. **Convener**, National conference on Chemical Physics (NCCP-2024) organized by the Department of Physics, Assam University, Silchar, during March 18-19, 2024 [Funded by SERB, CSIR, DRDO, and Assam University].
6. **Secretary**, International Conference on Systems and Processes in Physics, Chemistry and Biology (ICSPPCB-2023), March 02-04, 2023, organized by the Department of Physics, Assam University, Silchar.

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5. **Coordinator**, Virtual Workshop on Density Functional Theory and Its Applications (VWDFTIA-2021) organized by the Department of Physics, Assam University, Silchar, during September 8-12, 2021.
4. **Secretary**, International Conference on Systems and Processes in Physics, Chemistry and Biology (ICSPPCB-2018), March 01-03, 2018, organized by the Department of Physics, Assam University, Silchar [Funded by NEC Shillong, SERB, CSIR, RSC, ICTP, Italy and Assam Univ.].
3. **Coordinator**, Science Academies' Lecture Workshop on Atomistic Computer Simulation Techniques, 31st Oct-1st Nov. 2017, Physics Department, Assam University, Silchar.
2. **Convener**, National conference on Chemical Physics (NCCP-2017), during March 20-21, 2017 organized by the Department of Physics, Assam University, Silchar [Funded by SERB, CSIR, DRDO, BRNS, NEC Shillong and Assam University].
1. **Local Course-coordinator**, GIAN Program on Light scattering by different types of particles, with applications in Physics, April 05-13, 2016, at the Department of Physics, Assam University, Silchar.

### **12. Other Professional Activities:**

10. **Observer**, UGC-NET 2024 Exam conducted by National Testing Agency (NTA), New Delhi, at Silchar Centre.
9. **Observer**, CUET (UG) 2024 Exam conducted by National Testing Agency (NTA), New Delhi, at Silchar Centre.
8. **Member**, Board of Post Graduate Studies (BPGS), Department of Physics, Assam University, Silchar. (2024-2027)
7. **Observer**, NEET (UG) 2023 Exam conducted by National Testing Agency (NTA), New Delhi, at Silchar Centre.
7. **Observer**, CUET (PG) 2022 Exam conducted by National Testing Agency (NTA), New Delhi, at Silchar Centre.
6. **Member**, Board of Under Graduate Studies (BUGS), Department of Physics, Assam University, Silchar. (2022)
5. **Member**, Board of Post Graduate Studies (BPGS), Department of Physics, Assam University, Silchar. (2021-2024)
4. **Exam Coordinator**, End Semester Exam, Department of Physics, Assam University, Silchar. (August/September 2021)
3. **Member**, School Board, School of Physical Sciences, Assam University, Silchar. (2018-2020)
2. **Member**, Board of Post Graduate Studies (BPGS), Department of Physics, Assam University, Silchar. (2015-2018)
1. **Coordinator**, Departmental Admission Committee, M.Sc. (Physics) Entrance Exam, 2018.

### **13. Courses taught**

M.Sc. (Physics): Quantum Mechanics-I, Atomic and Laser Physics, Molecular Spectroscopy, Statistical Mechanics, Practical Labs, Ph.D. Course work

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### **Language Known**

Read, write and speak: English and Hindi

### **Member of Scientific Societies**

- Life Member of the Laser and Spectroscopic Society of India.
- Life Member of the Indian Science Congress Association.