

Dr. P. K. Shukla

Assistant Professor (Stage-II)

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1. Employment History

March 2014 – Present	Assistant Professor (Stage-II), Department of Physics, Assam University, Silchar, Assam, Teaching & Research.
March 2010 – March 2014	Assistant Professor (Stage-I), Department of Physics, Assam University, Silchar, Assam, Teaching & Research.
Aug. 2013 – July 2014	Raman Post Doctoral Fellow, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, U.S.A. Research, Advisor: Professor Jean-Luc Bredas.
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

2. Educational Background

2008 Ph. D. (Physics)	Banaras Hindu University, Varanasi – Title of Thesis- “ <i>Study of Electronic Structure, Properties, Interactions and Reactions of Some Biologically Important Molecules and Other Molecules</i> ”. Supervisor: Prof. P.C. Mishra, Physics Deptt., B.H.U., Varanasi. [Specific date of thesis submission: Dec. 31, 2008 and specific date of viva-voce: Feb. 14, 2010].
2002 M. Sc. (Physics)	VBS Purvanchal University, Jaunpur - First Division with 75.4% marks.
2000 B. Sc. (Physics, Chemistry and Mathematics)	VBS Purvanchal University, Jaunpur - First Division with 67.3% marks.
1997 Intermediate	U.P. Board Allahabad - First Division with 70.8% marks.
1995 High School	U.P. Board Allahabad - First Honours Division with 76.3% marks.

3. Awards/Fellowships

- ♦ INSA Visiting Scientist Award for 02 months for visiting Theoretical Sciences Unit, JNC SAR, Bengaluru. **Award Year: 2019**

- ◆ UGC Raman Fellowship for post-doctoral studies for one year at the Georgia Institute of Technology, Atlanta, U.S.A UGC Raman Fellowship for Post Doctoral Studies in USA under Indo-US 21st 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 “1st 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**]

4. Specialization & Research Interests: Chemical Physics, Biophysics

• Molecular electronic structure calculations	• Density functional theory (DFT)
• Structure and properties of biomolecules	• Carbon nanomaterials (CNTs and graphene-based materials)
• Biomolecular interactions and reactions	• Organic photovoltaics (OPV) materials
• DNA damage and repair	• Design and properties of ruthenium anticancer drugs
• Bulk and Specific Solvent effect	

5. List of Publications (* denotes corresponding author), h-index: 11

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, *Int. J. Quantum Chem.* **2007**, 107, 1270-1283.
2. **P. K. Shukla** and P. C. Mishra
H₂O₃ as a Reactive Oxygen Species: Formation of 8-Oxoguanine from Its Reaction with Guanine, *J. Phys. Chem. B* **2007**, 111, 4603-4615.
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, *Chem. Phys. Lett.* **2007**, 449, 323-328.
4. **P. K. Shukla** and P. C. Mishra

- Catalytic Involvement of CO₂ in the Mutagenesis Caused by Reactions of ONOO⁻ With Guanine, *J. Phys. Chem. B* **2008**, 112, 4779-4789.
5. **P. K. Shukla** and P. C. Mishra
Reactions of NO₂Cl with Imidazole: A Model Study for the Corresponding Reactions of Guanine, *J. Phys. Chem. B* **2008**, 112, 7925-7936.
6. Saumya Tiwari, **P. K. Shukla** and P. C. Mishra
Improved Electrostatic Properties Using Combined Mulliken and Hybridization- Displaced Charges for Radicals, *J. Mol. Model.* **2008**, 14, 631-640.
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, *Phys. Chem. Chem. Phys.* **2009**, 11, 8191-8202.
8. N. R. Jena, **P. K. Shukla**, H. S. Jena, P. C. Mishra and S. Suhai
O6-Methylguanine Repair by O6-Alkylguanine-DNA Alkyltransferase, *J. Phys Chem. B* **2009**, 113, 16285-16290.
9. **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**
10. **P. K. Shukla** and P. C. Mishra
A Quantum Chemical Study of Reactions of DNA Bases with Sulphur Mustard: A Chemical Warfare Agent, *Theor. Chem. Acc.* **2010**, 125, 269-278.
11. 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, *J. Phys. Chem. A* **2010**, 114, 97-104.
12. **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, *Chem. Phys.* **2010**, 369, 101-107.
13. 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, *Chem. Phys.* **2010**, 375, 118-129.
14. **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, *Int. J. Quantum Chem.* **2011**, 111, 2160-2169.
15. **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.

16. **P. K. Shukla**, Vinay Ganapathy and P. C. Mishra
A Quantum Theoretical Study of Reactions of Methyl diazonium Ion With DNA Base Pairs, *Chem. Phys.* **2011**, 388, 31-37.
17. **P. K. Shukla*** and P. C. Mishra
Base Pairing Patterns of DNA Base Lesion Spiroiminodihydantoin: A DFT Study, *Int. J. Quantum Chem.* **2013**, 113, 2600-2604.
18. 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, *Chem. Mater.* **2014**, 26, 2299-2306.
19. 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, *Int. J. Quantum Chem.* **2014**, 114, 1637-1644.
20. K. Bhattacharjee and **P. K. Shukla***
A Density Functional Theory Study of Methylation Reactions of CH_3N_2^+ with Guanylate and Deoxyguanylate, *Adv. Sci. Lett.* **2015**, 21, 2649-2652.
21. 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.
22. K. Bhattacharjee, P.C. Mishra and **P. K. Shukla***
Mechanism of Methylation of 8-Oxoguanine due to Its Reaction with Methyl Diazonium Ion, *Molecular Simulation* **2017**, 43, 196-204.
23. K. Bhattacharjee and **P. K. Shukla***
Does 8-Nitroguanine Form 8-Oxoguanine? An Insight from Its Reaction with $\bullet\text{OH}$ Radical, *J. Phys. Chem. B* **2018**, 122, 1852-1861.
24. K. Bhattacharjee and **P. K. Shukla***
A Theoretical Characterization of Reactions of HOOO Radical with Guanine: Formation of 8-Oxoguanine, *Struct. Chem.* **2018**, 29, 1109-1118.
25. S. Biswas, P.K. Shah and **P. K. Shukla***
Methylation of DNA Bases by Methyl Free Radicals: Mechanism of Formation of C8-Methylguanine, *Struct. Chem.* **2018**, 29, 1333-1340.
26. 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, *Struct. Chem.* **2020**, 31, 679-689.
27. P. K. Shah and **P. K. Shukla***
A DFT Study of Reactions of Ru(III) Anticancer Drug KP1019 with 8-Oxoguanine and 8-Oxoadenine, *Struct. Chem.* **2020**, 31, 2087-2092.

28. Z. 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.
29. Zeaul H. Mazumder, D. Sharma, D. Sengupta, A. Mukherjee, J. S. Boruah, S. Basu, **P. K. Shukla**, T. Jha
Photodynamic activity attained through raptured π -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.
30. B.I. Laskar and **P. K. Shukla***
Adsorption of HOOO $\cdot$ radical on pristine and doped graphene – A First-principles study, *Structural Chemistry* (2021). <https://doi.org/10.1007/s11224-020-01702-w>

6. Research Projects (Completed/Ongoing)

1. Project Molecular Mechanisms of Action of Ruthenium Anticancer Drugs: A Quantum Computational Study (SR/FTP/PS-047), **March 2015 - Sept. 2018**, Funded by Science and Engineering Research Board (SERB), Department of Science and Technology (DST), Govt. of India, New Delhi, Sanctioned budget: 19.39 lakh.

7. Research guidance

Ph. D.: completed – 01, ongoing – 04 **M.Phil.:** completed – 01

8. Courses taught

M.Sc. (Physics): Statistical Mechanics, Quantum Mechanics-I, Atomic and Laser Physics, Molecular Spectroscopy.

9. Invited Talks:

1. 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**.
2. 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. Molecular mechanisms of formation of mutagenic DNA lesions: A DFT study at the 2nd 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.
4. Molecular Mechanisms of Ruthenium Anticancer Drug – DNA Interaction at the 6th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2016) held during **Nov. 5-8, 2016** organized by the University of Lucknow, Lucknow, **India**.

5. 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**

10. Participation in seminars/conferences etc.

(A) International Seminars/Conferences

1. **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.
2. **Paper Presentation (Oral)** entitled “Theoretical Study of DNA Damage at Molecular Level” in the XXVII IUPAP International Conference on Computational Physics (CCP2015) held during **Dec. 2-5, 2015**, at the IIT Guwahati, Assam, **India**.
3. **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 **Jan. 10-12, 2015**, at the Department of Physics, Banaras Hindu University, Varanasi, U.P., **India**.
4. **Participated** in the Georgia Tech-COPE 10th Anniversary Symposium on **March 14, 2014** at the Georgia Tech Global Learning Center, Atlanta, **U.S.A.**
5. **Participated** in the Theoretical Chemistry Day Symposium on **Oct. 15, 2013** at the School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, **U.S.A.**
6. **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 Multidisciplinary Approach” organized during **Feb. 24-27, 2010** by University of Lucknow and Humboldt Academy Lucknow at the University of Lucknow, U.P., **India**.
7. **Paper Presentation (Poster)** entitled “CO₂ as a Catalyst in the Formation of 8-Oxoguanine and 8-Nitroguanine Due to Reaction of ONOO⁻ with Guanine: A DFT Study” in the 13th International Congress of Quantum Chemistry (13-ICQC) held during **June 22-27, 2009**, at the University of Helsinki, Helsinki, **Finland**.
8. **Paper Presentation (Poster)** entitled “Can H₂O₃ Oxidize Guanine Forming Mutagenic Product 8-Oxoguanine More Efficiently Than H₂O₂? 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 **Nov. 7-9, 2008**, at Department of Physics, B.H.U., Varanasi, **India**.

(B) National Seminars/Conferences

1. **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 **Feb. 13-15, 2010**, at the Department of Physics, Banaras Hindu University, Varanasi, U.P., **India**
2. **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 **Feb. 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 96th Indian Science Congress under “ISCA Young Scientists Award Programme” in the Section of Physical Sciences, held on **Oct. 17, 2008**, at the North Eastern Hill University, Shillong, Meghalaya, **India**.
4. **Paper Presentation (Oral)** entitled “A Quantum Chemical Approach to Oxidative Nature of H₂O₃: Formation of The Mutagenic Agent 8-Oxoguanine” in the 1st *One Day Conference on New Trends in Research*” held on **Oct. 27, 2007**, at the Department of Physics, Banaras Hindu University, Varanasi, U.P., **India**. University Level Conference.
5. **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**.

11. Participation in FDP/Workshops/etc.

1. **Attended** Faculty Development Programme on “Managing online classes and co-creating moocs: 2.0” from **May 18 – June 03, 2020**, organized by Teachers Training Centre, Ramanujan College, University of Delhi.
2. **Attended** the “*Refresher Course in Physics*” organized by the UGC-Human Resource Development Centre, University of Allahabad, Allahabad, during **Nov. 12-Dec. 02, 2018**.
3. **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**.
4. **Participated** in the Workshop on “*Statistical Physics of Soft Matter (SPSM-2015)*” held at the Department of Physics, B.H.U., Varanasi, **during Nov. 26-30, 2015**.
5. **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 from **May 19-23, 2014** in **Pittsburgh, PA, U.S.A.**
6. **Attended** the “*Refresher Course in Physics*” organized by the Academic Staff College-Kurukshetra University during **May 02-22, 2013**, at the Department of Physics, Kurukshetra Univ., Kurukshetra, Haryana, India.
7. **Attended** “*59th Orientation Course*” organized by the Academic Staff College-B.H.U., Varanasi during **January 03-30, 2012**.
8. **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 **Jan. 09-31, 2011**.

12. Professional Activities:

1. **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].
2. **Coordinator**, Science Academies' Lecture Workshop on Atomistic Computer Simulation Techniques, 31st Oct-1st Nov. 2017, Physics Department, Assam University, Silchar.
3. **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.].
4. **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.
5. **Member**, Board of Post Graduate Studies (BPGS), Department of Physics, Assam University, Silchar. (2015-2018)
6. **Member**, School Board, School of Physical Sciences, Assam University, Silchar. (2018-2020)
7. **Coordinator**, Departmental Admission Committee, M.Sc. (Physics) Entrance Exam, 2018.

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.

Personal Information

- **Full Name** Pradeep Kumar Shukla
- **Father's Name** Shri Jay Shankar Shukla
- **Date of Birth** July 20, 1981
- **Gender** Male
- **Marital Status** Married
- **Nationality** Indian
- **Permanent Address** Vill. & Post. – Kudda
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