CURRICULUM VITAE

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PERSONAL INFORMATION:

Date of Birth:	30.11.1971
Sex:	Male
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ACADEMIC QUALIFICATION:

M.Sc., Ph.D

Length of teaching experiences at UG level :	**17** years
Length of teaching experiences at PG level :	Less than one year
Length of research experiences :	**16** years
Length of research guidance at doctoral level experiences:	**4** years
No. of Ph.D students presently guiding :	**08** (eight)
No. of Ph.D students finally registered for Ph. D degree :	**03** (three)
No. of students awarded Ph.D degree :	**01** (one)
No. of students submitted Ph.D thesis:	**01** (one)
No. of research Paper Published:	**37** (thirty seven)
Total nos. of Seminar/Conferences attended:	
International	**02** (two)
National	**09** (nine)
Regional/Local /Others	**02** (two)

Projects: (ongoing/completed)

1. Effect of alkylation on DNA base pair: A Theoretical Approach

   Completed

   Funding agency UGC, New delhi
2. Density Functional and QM/MM Studies on Bisalkylating Anticancer Drug Molecules and Their Interaction with DNA

   Completed

   DST, New Delhi
3. QSAR analysis on few 9-aminoacridine Derivatives

   Ongoing

   UGC, New Delhi
4. DNA damage and degradation: A Density Functional Study,

   Ongoing

   DST, New Delhi

PUBLICATIONS:

BOOKS PUBLISHED:

1. **Molecular docking studies on polyphenolic compounds in Chemistry of Phenolic Compounds: State of the Art**, Ed. J.B. Baruah, Nova Science Publishers, Inc., New York, pp 131-139, **2011**.

2. ***Fundamentals of Quantum Chemistry***, Global Publishing House, India, **2013**.

3. ***Density Functional Studies of Bis-alkylating Nitrogen Mustards,*** **in Frontier in Computational Chemistry,** Vol 2 Ed. Zaheer Ul Haq, Jeffry, D. Madura, Bentham E-Books, UAE, pp 121-186, **2015**

List of Published Research Papers:

1. T. Thakuria, M.L. Das, **P. K. Bhattacharyya**, and C. Medhi, *Proton Induced Structual Reorganization of a Few Carbonyl Molecules in the Ground and Excited States*; *J. Chem. Inf. Comput. Sci.;* **1999**, 39, 267-71.

2. **P. K. Bhattacharyya**, and C. Medhi, *Ab initio calculation on the effect of substituents in the alkylation mechanism by nitrogen mustard at N-7 of guanine; Ind. J. Chem.;* **2004**, 43A, 2043-48.

3**. P. K. Bhattacharyya**, and C. Medhi, *Theoretical study on the mechanism of alkylation at N-7 of guanine by few nitrogen* mustard; *Ind. J. Chem.***; 2005**, 44B, 1319-23.

2007

4. M. Sharma, B. Sarma, **P. K. Bhattacharyya**, R. C. Deka and D. Dutta; *Dicarbonylrhodium(I) complexes of aminophenols and their catalytic carbonylation reaction*; *Appl. Organometal. Chem*.; **2007**, 21, 256-263.

5. **M. Karim,** P. K. Bhattacharyya **and C. Medhi;** ***Ionic effect on some anticancer drugs from analysis of their metal ion and proton affinities*****; *Ind. J. Chem***.; 2007, **46A, 1257-62**.

2010

6. D. Singh, **P. K. Bhattacharyya** and J. B. Baruah; *Structural Studies on Solvates of Cyclic Imide Tethered Carboxylic Acids with Pyridine and Quinoline*; *Cryst. Growth Des.*; **2010**, 10, 348–356.

2011

7. R. Sarma, **P. K. Bhattacharyya** and J. B. Baruah; *Short range interactions in molecular complexes of 1,4-benzenediboronic acid with aromatic N-oxides*; *Comput. Theoret. Chem.;* **2011**, 963, 141–147.

8. **P. K. Bhattacharyya** and R. Kar; *Does structural variation in the aziridinium ion facilitate alkylation?* Comput. *Theoret. Chem.;* **2011**, 967, 5-11.

9. N. Sarmah, B. Neog, and **P. K. Bhattacharyya**, *Affinity of aziridinium ion towards different nucleophiles: A density functional study*, *Comput. Theoret. Chem.;* **2011**, 976, 30–35.

10. B. Neog, N. Sarmah, R. Kar, and **P. K. Bhattacharyya**, *Effect of external electric field on aziridinium ion intermediate: A DFT study, Comput. Theoret. Chem.;* **2011**, 976, 60–67

2012

11. M. Borah, **P. K. Bhattacharyya** and P. Das, *Iron carbonyl complex containing bis[2-(diphenylphosphino)phenyl]ether enhancing efficiency in the palladium-catalyzed Suzuki–Miyaura reaction, Appl. Organometal. Chem*. **2012**, 26, 130-134.

12. B. Neog, N. Sarmah, R. Kar and **P. K. Bhattacharyya**, *Structural variation facilitate alkylation: A conceptual DFT study, Comput. Theoret. Chem.;* **2012**, 986, 79–84.

13. A. Tairai, **P. K. Bhattacharyya** and R. Kar, P. Das, *Primary amine-based palladium(II) complexes as catalysts for Suzuki-Miyaura reaction: Experimental and theoretical investigations on the effects of substituents on nitrogen atom, Ind. J. Chem.;* **2012**, 51A, 1545-1552.

2013

14. B. Neog, S. Sinha and **P. K. Bhattacharyya**, *Alkylation of DNA by nitrogen mustards: A DFT study, Comput. Theoret. Chem.;* **2013,** 1018, 19-25.

15. R. J. Sarma, A. K. Deka and **P. K. Bhattacharyya**, *Coordination of Bromide Anions and Organic Bromine to Tryptophan Ligands, J. Mol. Struct.*, **2013**, 1052, 197–203.

16. B. Neog, N. Sarmah, S. Sinha and **P. K. Bhattacharyya**, *Density functional based reactivity studies on aziridinium ion intermediate; J. Ind. Chem. Soc.*, **2013**, 90, 2231-2236.

17. N. Ahmed, **P. K. Bhattacharyya** and S. K. Bhattacharjee, Synthesis and Antibacterial Activity of Benzo-2-phenyl-1-thia-2, 3-diazolium bromide and its Derivatives, *Int. J. Chemistry*, **2013,** 2, 427-435

2014

18. S. Sinha and **P. K. Bhattacharyya**, *Alkylation of guanine by formononetin nitrogen mustard derivatives: A DFT Study, Comput. Theor. Chem*. **2014**, 1027, 135–141

19. S. Sinha and **P. K. Bhattacharyya**, *Variation of reactivity of aziridinium ion during alkylation Mol.Phys.*, **2014**,112, 14-21.

20. K. K. Bania, A. K. Guha, **P. K. Bhattacharyya** and Sourab Sinha, *Effect of Substituent and Solvent on Cation-π Interaction in Benzene and Borazine: A Computational Study***,** *Dalton Transactions*, **2014**, 43, 1769-1784.

21. B. Neog, N. Sarmah and **P. K. Bhattacharyya**, *Effect of external electric field on drug-guanine adduct: A conceptual density functional theory study, J. Ind. Chem. Soc.;* **2014,** 91, 95-99.

22. S. Sinha, B. Neog, N. Sarmah and **P. K. Bhattacharyya**, *Effect of guanine alkylation on Keto-enol tautomerism: A DFT study, J. Ind. Chem. Soc.*, **2014**, 91, 679-687

23. N. Sarmah, **P. K. Bhattacharyya** and K. K. Bania, Substituent and Solvent Effects on the Absorption Spectra of Cation-π Complexes of Benzene and Borazine: A Theoretical Study, *J.Phy. Chem. A*, **2014**, 118, 3760–3774

24. C. Tamuly, M. Hazarika, M. Bordoloi, **P. K. Bhattacharyya** and Rahul Kar, Biosynthesis of Ag nanoparticles using pedicellamide and its photocatalytic activity: an eco-friendly approach, *Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy*, **2014**, 132, 687–691

25. B. J. Dutta and **P. K. Bhattacharyya**, Reactivity and Aromaticity of Nucleobases are Sensitive Towards External Electric Field, *J.Phy. Chem. B,* **2014**, 118, 9573−9582.

26. N. Ahmed, S. K. Bhattacharjee and **P. K. Bhattacharyya**, Comparative study on nucleophilic/electrophilic behaviours of divalent organosulfur compounds: A DFT study, *J. Ind. Chem. Soc.*, **2014**, 91, 1171-1183.

27. J. Sarma, S. Sinha, N. Sarmah, S. K. Purkayastha, P. Sarkar and **P. K. Bhattacharyya** DFRT studies of amide-coupled benzoic nitrogen mustard derivatives, *J. Ind. Chem. Soc.*, **2014,** 91, 2211-2216**.**

2015

28. K. Baruah, S. Sinha, S. Hazarika and **P. K. Bhattacharyya**, QM/MM Studies on Cyclodextrin-Alcohol Interaction, *Journal of Macromolecular Science, Part A, Pure and Applied Chemistry,* **2015,** 52, 64–68.

29. B. C. Deka and **P. K. Bhattacharyya**, Understanding Chitosan as A Gene Carrier: A DFT Study, *Comput. Theor. Chem*. **2015**, 1051 35–41.

30. J. Kumar, **P. K. Bhattacharyya** and D. K. Das, New duel fluorescent "on-off" and colorimetric sensor for Copper(II): Copper(II) binds through N coordination and pi cation interaction to sensor, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **2015**, 138, 99–104

31. **P. K. Bhattacharyya**, Effect of External Electric Field on Ground and Singlet Excited States of Phenylalanine: A Theoretical Study, *Comput. Theoret. Chem.*, **2015**, 1057, 43-53.

32. P. P. Biswas, **Pradip K. Bhattacharyya** and D. K. Das, Synthesis, characterization, DFT/TDDFT calculation and superoxide dismutase activity of copper(II) complex with ligand derived from benzil and cysteine, *J. Chem. Pharma. Res.*, **2015**, 7, 102-108

33. B. Sarma, **P. K. Bhattacharyya** and D. K. Das, Synthesis, characterization and superoxide dismutase activity of bi-copper (II)-bisacetato- phthalicacid[bis (benzyloxy)ethyl]ester, *J. Chem. Sci.* **2015**, 127, 455–459.

34. **P. K. Bhattacharyya**, Reactivity, Aromaticity and Absorption Spectra of Pillar[5]arene conformers: A DFT Study, *Comput. Theoret. Chem.*, **2015**, 1066 20–27.

35. R. K. debnath, A. Kalita, S. Sinha, **P. K. Bhattacharyya**, B. Mondal, J. N. Ganguli, Solvent dependent disproportion of Cu(II) complexes of N2O2 ligands: direct evidence of formation of phenoxyl radical: an experimental and computational study, *Asian Journal of Chemistry*, **2015**, 27, 4490–4500

36. B. J. Dutta and **P. K. Bhattacharyya**, DFT Studies on Hydrogen-bonding, Stacking and X-H$\cdots\pi$ Bonded Systems in Presence of External Electric Field, *Int. J. Quant. Chem*, **2015**, 115, 1459-1466.

37. K. Baruah, **P. K. Bhattacharyya**, Effect of external electric field on Cyclodextrin-Alcohol adducts: A DFT study, *J. Chem. Sci.* **2015,** 127, 1109–1117.

38. K. Baruah, **P. K. Bhattacharyya,** S. Hazarika**,** Adsorption of Dilute Alcohols onto Cyclodextrine-Polysulfone Membrane : Experimental and Theoretical Analysis, *J. Chemical & Engineering Data***, 2015,** 60, 2549–2558**.**

39. S. Sarma, **P. K. Bhattacharyya**, D. K. Das, New Fluorescent "Off-On" Sensor for Al^{3+} Derived from L-alanine and Salicylaldehyde, *J Fluoresc*, **2015**, 25, 1537-1542.

40. J. Deka, L. Satyanarayana, G. V. Karunakar, **P. K. Bhattacharyya** and K. K. Bania, Chiral modification of copper exchanged zeolite-Y with cinchonidine and its application in asymmetric Henry reaction, *Dalton Trans.*, **2015**, 44, 20949-63.

2016

41. B. C. Deka and **P. K. Bhattacharyya**, Response of Chitosan-Nucleobase interaction towards external perturbations: A Computational study, *Comput. Theoret. Chem.*, **2016**, 1078, 72–80**.**

42. S. K. Purkayastha and **P. K. Bhattacharyya**, Does oligomerization in fused thiophene affects reactivity and aromaticity?, *J. Chem. Sci*. **2016**, 128, 1-14.

43. **P. K. Bhattacharyya**, A DFT study on reactivity, aromaticity and absorption spectra of perylo[1,12-b,c,d] thiophene tetraester doped with B, N, O, Se and BN, *Comput. Theor. Chem.* **2016**, 1082, 29–40

44. B. Banik, A. Tairai, **P.K. Bhattacharyya**, Pankaj Das, Excellent Suzuki-Miyaura activity catalyzed by a new Pd(II) complex with sulfonamide-Schiff base ligand, *Appl. Organometal. Chem*. **2016**, 30, 519–523.

45. S. Sarma, **P. K. Bhattacharyya**, D. K. Das, Condensation Product of Phenylalanine and Salicylaldehyde: Fluorescent Sensor for Zn^{2+}, *J Fluorescence*, **2016,** 26, 899-904.

46. B. C. Deka, **P. K. Bhattacharyya**, Reactivity of chitosan derivatives and their interaction with guanine: A computational study, *J. Chem. Sci.* **2016**, 4, 589-598.

47. B. Saha, **P. K. Bhattacharyya**, Adsorption of amino acids on boron and/or nitrogen doped functionalized graphene: A Density Functional Study, *Comput. Theor. Chem.* 2016, 1086, 45–51

48. S. P. Mahanta, B. Dutta, **P. K. Bhattacharyya** and K. K. Bania, Cation-π Interaction in Molecular Dyads: A DFT and TDDFT Study, *RSC Adv.*, **2016**, 6, 63827-63836.

49. B. C. Deka, S. K. Purkayastha, H. Sharma and **P. K. Bhattacharyya**, Ground and Excited States of Neutral and Cationic Thieno[3,2-b]thiophene: A DFT Study, *Comput. Theor. Chem.* **2016**, 1091, 41–48.

50. B. Saha and **P. K. Bhattacharyya**, Understanding reactivity, aromaticity and absorption spectra of carbon cluster mimic to graphene: a DFT study, *RSC Adv*., 2016, 6, 79768–79780

51. B. C. Deka, S. K. Purkayastha and **P. K. Bhattacharyya**, Formation of thiophene sandwiches through cation–π interaction: A DFT study, *Comput. Theor. Chem.* 2016, 1095, 83–92.

52. H. Sharma, B. C. Deka and **P. K. Bhattacharyya**, Behaviour of Potential Energy Surface of C–X Bonds in Presence of Solvent and External Electric Field: A DFT Study, *J Theor. Compt. Chem.* 2016, 15, 1650051-19.