



Arya Vidyapeeth College
আর্য্য বিদ্যাপীঠ মহাবিদ্যালয়



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Date of joining the present service: 25-10-2017 (As principal)

Academic Qualification MSc, PhD

Teaching Experience

In UG level: 22 years

In PG level: 3 years



Research Date of obtaining / PhD Degree: 2005, Gauhati University
 Experience Title of the PhD thesis:
 “THEORITICAL STUDIES OF SOME ANTICANCER DRUGS”
 Length of research experience: 15 years
 Specialization (Area of interest) computational Chemistru
 Research Guidance (PhD guideship): From Gauhati University
 No. of student obtained PhD degree: 06
 No. of student perusing PhD degree: 05
 No. Of research projects:

Title of the project	Funding agency	Amount (in Rs)	Status (ongoing/completed)
Effect of alkylation on DNA base pair: A Theoretical Approach.	UGC	85,000/-	Completed
QSAR analysis on few 9-aminoacridine Derivatives.	UGC	6,05,000/-	Completed
Density Functional and QM/MM Studies on Bisalkylating Anticancer Drug Molecules and Their Interaction with DNA.	DST	12,95,000/-	Completed
DNA damage and	DST	21,43,000/-	Completed

degradation: A Density Functional Study			
Computational Studies on the weak interactions.	DST (Matrices)	6,60,000/-	Ongoing

Publications

No. Of Books authored: 01

Fundamentals of Quantum Chemistry, Global Publishing House, India, 2013, 978-93-81563-17-5

No. Of Book chapters published: 02

“Density Functional Studies of Bis-alkylating Nitrogen Mustards” In Frontiers In Computational Chemistry, Zaheer Ul-Haq and Jeffry D. Madura Eds. Vol 2, 2015, ISBN 978-1-60805-979-9

“Molecular Docking studied on Polyphenolic Compounds” in Chemistry of Phenolic Compounds: State of the Art, Ed. J.B. Baruah Eds., Nova Science Publishers, Inc., New York, 2011, ISBN 978-1-61122-099-5

No. Of Research paper published: 80

Published Papers:

1. M. J. Baruah, M. Sharma, B. Das, P. Saikia, L. Saikia, S. Roy, G. V. Karunakar, **P. K. Bhattacharyya**, K. K. Bania, Boosting multiple photo-assisted and temperature controlled reactions with a single redox-switchable catalyst: Solvents as internal substrates and reducing agent, *Journal of Catalysis*, **2020**, 388, 104–121
2. Self pH Regulated Iron(II) Catalyst for Radical Free Oxidation of Benzyl Alcohols, B. Das, M. J. Baruah, M. Sharma, B. Sarma, G. V. Karunakar, L. Satyanarayana, S. Roy, **P. K. Bhattacharyya**, K. K. Bania, *Applied Catalysis A, General*, **2020**, 589, 117292
3. M. Sharma, B. Das, M. J. Baruah, **P. K. Bhattacharyya**, L. Saikia, and K. K. Bania, Pd-NiO-Y/CNT Nanofoam: A Zeolite-Carbon Nanotube Conjugal

Exhibiting High Durability in Methanol Oxidation, Chem Comm, *Chem. Commun.*, **2020**, 56, 375-378

4. B. Saha and **P. K. Bhattacharyya**, DFT study on the formation of homo and hetero dimers of BN-doped tetracyclic fused aromatics via $\pi\cdots\pi$ stacking, *Chemistry Select*, **2019**, 4, 481-91.

5. B. Saha, **P. K. Bhattacharyya**, Anion $\cdots\pi$ interaction in oxoanion-graphene complex using coronene as model system: A DFT study, *Comput. Theor. Chem.* **2019**, 1147, 62–71.

6. B. Saha, H. Sharma and P. K. Bhattacharyya, Non-classical B-H_b $\cdots\pi$ interaction in Diborane \cdots localized- π sandwiches: A DFT study, *Int. J. Quant. Chem.*, **2019**, 20, e25998

7. N. Sharmah and **P. K. Bhattacharyya**, Cation mediated sandwich formation between benzene and pillar[5]arene: A DFT study, *Mol. Physics*, 2019, 117, 734-45.

8. B. Saha and **P. K. Bhattacharyya**, B-H_b $\leftarrow\cdots$ X (X= N, O, P, S, F, Cl, Br) interactions—A density functional study, *Int. J. Quant. Chem.*, **2018**, 118, e25654.

9. B. C. Deka and P. K. Bhattacharyya, A density functional study on synthetic polymer-amino acid interaction, *J. Chem. Sci.* **2018**, 130:122.

10. H. Sharma, B. C. Deka, B. Saha and **P. K. Bhattacharyya**, Understanding the structure, reactivity and absorption spectra of borazine doped pillar[5]arene: A DFT study, *Comput.Theor.Chem.* **2018**, 1139, 82-89.

11. B. Saha, S. Sinha, H. Sharma and **P. K. Bhattacharyya**, On the Formation of Polymeric Housene Molecules of Group 15 Elements (N, P, As and Sb): A DFT Study, *J. Phy. Chem.A*, **2018**, 122, 6780-6788.

12. B. Saha, R. Deka, A. Das and **P. K. Bhattacharyya**, On the formation of sandwich and multidecker complexes via $\pi\cdots\pi$ interaction: A DFT study, *New J. Chem.*, 2018, 42, 19924-19933.

13. B. Saha and **P. K. Bhattacharyya**, A density functional study on the adsorption of 5-membered N-heterocycles on B/N/BN doped graphene: Coronene as a model system, *ACS OMEGA*, **2018**, 3, 16753-16768.

14. **P. K. Bhattacharyya**, B-H_b $\cdots\pi$ Interaction in Benzene-borazine Sandwich and Multidecker Complexes: A DFT Study, *New J. Chem.*, **2017**, 41, 1293–1302.

15. J. Kumar, A.Bhowmick, S.Banu, **P.K. Bhattacharyya**, D.K.Das, 2-Hydroxyacetophenone and ethylenediamine condensed Schiff base: Fluorescent sensor for Al^{3+} and PO_4^{3-} , biological cell imaging and inhibit logic gate, *Inorganica Chimica Acta*, **2017**,462, 167-173.
16. B. C. Deka and **P. K. Bhattacharyya**, DFT study on host-guest interaction in chitosan-amino acid complexes, *Comput.Theor.Chem.* **2017**, 1110, 40-49.
17. **P. K. Bhattacharyya**, Exploring cation- π interaction in the complexes with $\text{B}\equiv\text{B}$ Triple Bond: A DFT study, *J.Chem.Phys A*, **2017**, 121, 3287-3298.
18. B. J. Dutta, N. Sarmah, **P. K. Bhattacharyya**, On the Effect of External Perturbation on Amino Acid Salt Bridge: A DFT Study, *J. Chem. Sci*, **2017**, 129, 533-541.
19. B.Saha and **P. K. Bhattacharyya**, B-H \cdots π interaction in borane-graphene complexes: Coronene as a case study, *New.J.Chem.* **2017**, 41, 5040-5054.
20. B. C. Deka and **P. K. Bhattacharyya**, Nitrogen Mustards: The Novel DNA Alkylator, *Clinical Cancer Drugs*, **2017**, 4(1), 10-46.
21. N. Sarmah, B.C. Deka and **P. K. Bhattacharyya**, Exploring cation- π interaction in half sandwiches and sandwiches with $\text{X}\equiv\text{X}$ triple bonds (X= C, Si and Ge): A DFT study, *Comput.Theor. Chem.* **2017**, 1115, 106–113.
22. S.Sinha and **P. K. Bhattacharyya**, Understanding the Influence of External Perturbation on Aziridinium ion Formation, *Mol.Phys.* **2017**, 116, 29-43.
23. H. Sharma and **P. K. Bhattacharyya**, Association of phenylboronic acids with hydrogen bond acceptors to form hydrogen bonded DD•AA type complexes: A DFT study, *New.J.Chem*, **2017**, 41, 10112–10120.
24. Sanchay J. Bora, Rima Paul, Mithun Nandi, **P. K. Bhattacharyya**, Two-fold interpenetrating btc based cobaltous coordination polymer: A promising catalyst for solvent free oxidation of 1-hexene, *J. Solid State Chemistry*, **2017**, 256, 38–44.
25. Himakshi Sharma, Bapan Saha, Pradip K Bhattacharyya, Sandwiches of N-doped Diamondoid and Benzene via Lone Pair cation and Cation- π Interaction: A DFT study, *New J. Chem*, **2017**, 41, 14420-14430.
26. 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.

27. S. K. Purkayastha and **P. K. Bhattacharyya**, Does oligomerization in fused thiophene affects reactivity and aromaticity?, *J. Chem. Sci.* **2016**, 128, 1-14.
28. **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.
29. B. Banik, A. Tairai, **P.K. Bhattacharyya**, Pankaj Das, Excellent Suzuki-Miyaura activity catalyzed by a new Pd(II) complex with sulphonamide-Schiff base ligand, *Appl. Organometal. Chem.* **2016**, 30, 519-523.
30. 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.
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32. 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
33. 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.
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35. 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.
36. 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
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38. N. Sarmah and **P. K. Bhattacharyya**, Behaviour of cation- π interaction in presence of external electric field. *RSC Adv.*, **2016**, 6, 100008–15.
39. K. K. Bania, A. K. Guha, **P. K. Bhattacharyya**, DFT and TDDFT study on cation- π complexes of diboryne ($\text{NHC} \rightarrow \text{B} \equiv \text{B} \leftarrow \text{NHC}$), *J. Chem. Phys.*, **2016**, 145, 184112.
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45. 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
46. 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.
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48. 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
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51. 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.
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55. S. Sinha and **P. K. Bhattacharyya**, Variation of reactivity of aziridinium ion during alkylation *Mol.Phys.*, **2014**, 112, 14-21.
56. 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.
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Borazine: A Theoretical Study, *J. Phy. Chem. A*, **2014**, 118, 3760-3774.

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61. 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.

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

Papers presented in Seminar/Conference	<ol style="list-style-type: none"> 1. National Seminar on Recent Aspects of Chemistry Education and Research, 2012, Department of Chemistry, Gauhati University, Guwahati, India, Sponsored by DST 2. National Symposium on Current Trends in Computational Chemistry, 2012, Department of Chemistry, North-East Hill University, Shillong, Sponsored by DST,UGC,CSIR, NEHU 3. Emerging trend in chemical sciences, 2012, Department of Chemistry, Gauhati University, Guwahati, India, Sponsored by UGC 4. First Indo-US workshop on Mathematical Chemistry, 1998. Visva-Bharati University, West Bengal, India, International. Sponsored by University of Minnesota, USA, CSIR, Visva Bharati, DST 5. National Seminar on Frontier Areas of Research in Chemistry, 2011, Department of Chemistry, Cotton College, Guwahati, India, Sponsored by UGC 6. National Seminar on Recent Advances in Synthesis and Catalysis, 2011, Department of Chemistry, Dibrugarh University, Dibrugarh, India, Sponsored by DST, CSIR, INSA,UGC
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Linkage with other institution (research collaboration)	<ol style="list-style-type: none"> 1. IITG 2. Tezpur University 3. Dibrugarh University 4. NEIST, Jorhat, Assam
Membership in reputed national/international agency	Member of Chemical Research Society of India