Curriculum vitae

Name: Dr. Amit Kumar Paul

Designation: Associate Professor

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Mailing Address:

Office: Department of Chemical Sciences
Bose Institute
Unified Academic Campus
EN 80, Sector V, Salt Lake City
Kolkata 700091

Permanent Address: 6, Joy Narayan Tarka Panchanan Lane, Kolkata - 700011

e-mail: amit.kp13@gmail.com, amit.paul@jcbose.ac.in

Date of Birth: 16th October, 1982

Sex: Male

Marital Status: Married

Nationality: Indian

Educational Qualification:

B. Sc. (Hons. in Chemistry, 1st Class, 63.5%), University of Calcutta, 2005.
M. Sc. (Specialization in Physical Chemistry, 1st Class, 73.2%), University of Calcutta, 2007.
Ph. D. (Science), IACS, Kolkata, University of Calcutta, January - 2013.

Title of Thesis: Beyond Born – Oppenheimer theories and it's implication to quantum dynamics

Employment Details

Sl. No.	Duration	Position
1	February 2013 – June 2016	Post doctoral Research Associate at Texas Tech University
2	June 2016 – November 2017	Assistant Professor (consolidated pay), NIT Meghalaya
3	November 2017 – September 2019	Assistant Professor Grade II, NIT Meghalaya
4	September 2019 – December 2023	Assistant Professor Grade I, NIT Meghalaya
5	December 2023 – May 2024	Associate Professor, NIT Meghalaya
6	May 2024 – till date	Associate Professor, Bose Institute

Award and Fellowship:

(a) Qualified the Graduate Aptitude Test in Engineering **(Gate 2007)**

(b) Qualified the National Eligibility Test (**NET 2007**) under CSIR fellowship

(c) Selected for OCES-2007 (IGCAR) at BARC, Mumbai

(d) International travel reward (including TA, DA and accommodation) from XXIst International Symposium on the Jahn-Teller Effect 2012, Japan

(e) Popular Poster award at XXIst International Symposium on the Jahn-Teller Effect, 2012

(f) Postdoctoral fellowship (**February, 2013- June, 2016**) by AFOSR grant, Texas Tech University, Texas, USA

(g) Visiting Scholar, University of Pisa, Italy, 2014.

(h) Fellow of Indian Chemical Society (Fellow no. F/8219)

(i) **Guided the Best M.Sc. thesis of NIT Meghalaya in 2021-22. (Awarded to Mr. Partha Pratim Borah, M.Sc. 2020-22**.

(j) **Excellent research contribution Award for the year 2021-22 at NIT Meghalaya**

(k) **Member of the Editorial Board, Int. J. Chem. Kinet.**

(l) **Guided the Best M.Sc. thesis of NIT Meghalaya in 2022-23. (Awarded to Ms. Prerana Bakli, M.Sc. 2021-23**.

Ph.D. Supervisor: Dr. Satrajit Adhikari, Senior Professor,
School of Chemical Sciences,
Indian Association for the Cultivation of Science,
2A & 2B Raja S. C. Mullick Road, Jadavpur
Kolkata – 700032, West Bengal, India

Postdoc Supervisor: (Late) Dr. William L. Hase
Paul Whitfield Horn Professor, Robert A. Welch Professor,
Department of Chemistry and Biochemistry,
Texas Tech University, Lubbock, TX 79409

Disciplines of research experiences:

(a) Chemical dynamics simulation with force field development by fitting *ab initio* interaction energy for several different orientations to the two body potential term.

(b) Condensed phase MM/MM and QM/MM simulation to study energy transfer processes

(c) Unimolecular Reaction dynamics

(d) Machine learning techniques for chemical dynamics simulations.

(f) Effect of anharmonicity in the reaction dynamics: A Monte Carlo Approach

(g) Parameterization of Potential Energy Surfaces into two-body interaction using genetic algorithm

(h) Theoretical development of beyond Born -Oppenheimer treatment, analytical expressions for non -adiabatic coupling elements (NACTs), their Curl-Divergence Equation and formulation of beyond Born – Oppenheimer equation.

(i) Calculation of Potential Energy Surfaces (PESs) and Non-adiabatic coupling elements (NACTs) using quantum chemistry calculations.

(j) Formulation of Diabatic PESs from Adiabatic representation of Schrödinger Equation following adiabatic to diabatic transformation (ADT) scheme.

(k) Quantum dynamics to obtain autocorrelation function and Fourier transformation of that function to obtain photoabsorption spectra.

Current research interest:

(a) Gas phase simulations on unimolecular, bimolecular systems, and their reaction dynamics

(b) Condensed phase calculation for various chemical reactions including solvent interaction based on QM/MM and MM/MM methodologies

(c) Machine Learning implementation of various chemical dynamics problems, particularly, in identifying the role of normal modes in chemical reactions

(d) Excited state dynamics of molecular systems using both adiabatic and non-adiabatic protocols and experimental collaborations.

Numerical calculation skills:

(a) *ab initio* calculations: MOLPRO, GAUSSIAN, NWChem
(b) Quantum dynamics: FFT – Lancoz, Chebyshev, DVR, Time-dependent DVR.
(c) Chemical Dynamics Package: VENUS
(d) Semiempirical Package: MOPAC
(e) Parameterization of PESs: GAfit
(f) Programming language: FORTRAN

Sponsored Projects:

Sl. No.	Title	Sponsoring Agency	Amount Sanctioned	Duration
1.	QM + MM Chemical Dynamics on Chemical Reactions and Non-Adiabatic Processes in Condensed Phase Molecular Systems	SERB-DST (ECR)	₹ 36,58,000/-	July, 2018 - January, 2022
2.	Post Transition State Dynamics on Chemical Reactions and the Effect	CSIR	₹ 13,96,000/-	August 2019- August 2022

	of Solvation			
3	On-the-Fly Chemical Dynamics Simulations in Gas and Condensed Phase Molecular Systems Using Machine Learning Approach	SERB-DST (CRG)	₹ 48,11,400/-	December 2022 – December 2025

Teaching and Supervising Experiences:

From	***To***	***Courses Taught***	***M.Sc. Project guided***	***Ph.D. guided***	***Postdoc guided***
Aug. 2016	Till Date	1. Quantum Mechanics, 2. Chemical Kinetics, 3. Molecular Spectroscopy, 4. Computational Chemistry, 5. Group Theory 6. Environmental Science	16 (completed) 2 (ongoing)	04 6(ongoing)	1 NPDF (ongoing)

Ph.D. Degree Awarded:

Sl. No.	**Name**	**Date of Degree**	**Title of the Thesis**	**Current Position**
1	Dr. Himashree Mahanta	23/05/2022	The Understanding of the Intramolecular Interactions in Aromatic Complexes through Computational Investigations of Unimolecular Dissociation and Association Reactions	Assistant Professor, Assam Kaziranga University
2	Dr. Sk. Samir Ahamed	05/09/2022	Molecular Dynamics Simulation on Energy Transfer and Chemical Reactions in Single/Mixed Bath Molecular Systems	Post-doctoral Fellow, University of Hawaii, USA
3	Dr. Ankita Agarwal	21/05/2024	Post-Transition State Dynamics on Ozonolysis of Catechol in Gas and Condensed Phase	Assistant Professor, Galgotias University, Greater Noida, UP
4	Dr. Palash Jyoti Boruah	05/12/2024	Investigations on the Reaction Mechanism of Chemical Reactions Based on Electronic Structure Calculations and Excited State Dynamics	Research Associate, IIT Guwahati

Conferences, Seminars, Workshops, etc. Organized

Sl. No.	Name of the Conference/Seminar/Workshop	Duration	Role	Status
1	Recent Advances in Chemistry (RAC 2019)	Oct. 12-13, 2019	Convener	National
2.	One Day workshop on Theoretical and Computational Chemistry	March 13, 2021	Convener	National
3.	Recent Advances in Chemistry: Theoretical and Computational Aspects 2022	November 18-20, 2022	Convener	National
4.	Interdisciplinary Horizons of Physical Chemistry	July 17 – 19, 2025	Jt. Convener	National

Invited Talks Delivered

1. Department of Chemistry, IITB
June 16th, 2015

2. Department of Chemistry, IIT-BHU
August, 8, 2015

3. Endothermic BRI review meeting by AFOSR, USA, 5th November, 2015, Dayton, OH, USA

4. School of Chemistry, University of Hyderabad
February 16, 2016

5. S. N. Bose National Centre for Basic Sciences, Kolkata
February, 26, 2016

6. National Conference on Chemical Physics (NCCP-2017), Assam University, Silchar, March 2017

7. Recent Trends in Chemical Science (RTCS 2017), NIT Meghalaya, Oct. 2017

8. SDMC 2018, Dooars, West Bengal, Feb. 2018.

9. IACS conference on Electronic Structures, Spectroscopy, and Dynamics, IACS, Kolkata, Feb, 2018

10. Department of Chemistry, IISER Mohali, May, 2018.

11. SDMC webinar

12. Theoretical Chemistry Symposium 2021, IISER Kolkata, SNBNSBS, SINP, IACS (online)

13. Theoretical Chemistry Meeting: Structure and Dynamics (TCMSD-2022)
26th - 29th May, 2022, IACS, Kolkata, India

14. Invited talk in the workshop on High Performance Computing and it's Multidiciplinary Applications, NIT Meghalaya, August 22 – 27, 2022

15. Invited Young Scientist Lecture in ETCS 2023, NEHU, 2 – 4 March 2023

16. Invited Talk in MS-TPCCP at IIT-B, 29-30 July 2023

17. Resource person talk at Refresher Course in Chemistry at NEHU, 5th August 2023

18. Invited talk at MS-PCCP in IIT Bombay, July 29-30, 2023.

19. Invited talk at IC-SDSS 2023, IACS, October 5-8, 2023.
20. Invited talk at QSCP, Jaipur, 14-20 October, 2023
21. Invited talk at SoPhyC Inaugural conference, IIT Kanpur, 29 – 31 October 2023
22. Invited hot topic talk at iCOMET, Jaipur, November 12 – 16, 2023
23. Invited Talk at SDMC 2024, Kaziranga, Feb. 22-25, 2024
24. Invited talk at RTCST 2024, IIT Patna, March 1-2, 2024
25. Invited talk at Machine Learning workshop at NIT Durgapur, March 3, 2024
26. Invited talk at FICS 2024 at IIT Guwahati, 2-4 December 2024
27. Invited talk at PCAMC 2024 at IISER-Kolkata, 11 - 14 December 2024
28. Invited Talk at Dept. of Chemistry, SVNIT, Surat. Organized by Chemshashtra student chapter, February 8, 2025
29. Invited Talk at the Dept. of Chemistry, IIT Bombay, March 4, 2025.
30. Invited Talk at NSRSSOF 2025 at Alipurduar University, March 25, 2025.
31. Invited Talk at the Dept. of Chemistry, University of North Bengal, March 26, 2025.
32. Invited Talk at Symposium on Recent Advances in Physical Chemistry Research (SRAPCR 2025), IACS, April 10-13, 2025.
33. Invited Talk at Bhawanipur Education Society College, June 09, 2025.
34. Invited Talk at Interdisciplinary Horizons of Physical Chemistry (IHPC 2025), Bose Institute, July 17-19, 2025.
35. Invited Talk at Advanced Materials & Technologies for Sustainable Energy & Future, 2025 (AMTEF-25), University of North Bengal, September 19-21, 2025.
36. Invited Talk at Society of Physical Chemistry Conference (SoPhyC 2025), IIT Patna, October 11-14, 2025.
37. Invited Talk at Recent Advances in Chemistry (RAC 2025), NIT Meghalaya, October 30 - November 1, 2025
38. Invited Talk at Computational Physics and Cyber Secure IT infrastructure, Amity University, Kolkata, 20-21, November 2025
39. Invited Talk at TCS 2025, IIT Bombay, 2-5 December 2025
40. Expert Lecture in the Refresher Course on *Chemistry for Sustainable Future* from December 9-22, 2025

Complete List of Publications

1. A quantum - classical approach to the molecular dynamics of butatriene cation with a realistic model Hamiltonian,
S. Sardar, **A. K. Paul**, P. Mondal, B. Sarkar and S. Adhikari,
Phys. Chem. Chem. Phys. **10**, 6388 (2008).
Impact Factor: **4.198**

2. The multi state multi mode vibronic dynamics of benzene radical cation with a realistic model Hamiltonian using a parallelized algorithm of quantum classical approach,
S. Sardar, **A. K. Paul**, R. Sharma and S. Adhikari,
J. Chem. Phys. **130**, 144302 (2009).
Impact Factor: **3.122**

3. A parallelized quantum - classical approach to explore the photo absorption spectrum of allene radical cation,
S. Sardar, **A. K. Paul** and S. Adhikari,
Mol. Phys. **107**, 2467 (2009).
Impact Factor: **1.642**

4. Photodissociation of H_2^+ upon exposure to an intense pulsed photonic Fock state,
A. K. Paul, S. Adhikari, Debasis Mukhopadhyay, G. J. Halász, ´ A. Vibók, Roi Baer and Michael Baer,
J. Phys. Chem. A **113**, 7331 (2009).
Impact Factor: **2.883**

5. Single surface beyond Born - Oppenheimer equation for a three state model Hamiltonian of Na_3 cluster,
A. K. Paul, S. Sardar, B. Sarkar and S. Adhikari,
J. Chem. Phys. **131**, 124312 (2009).
Impact Factor: **3.122**

6. H_2^+ photodissociation by a intense pulsed photonic Fock state,
A. K. Paul, S. Adhikari, R. Baer and M. Baer,
Phys. Rev. A. **81**, 013412 (2010).
Impact Factor: **2.991**

7. Space - Time contours to treat intense field - dressed molecular states,
A. K. Paul, S. Adhikari, and M. Baer,
J. Chem. Phys. **132**, 034303 (2010).
Impact Factor: **3.122**

8. Single surface beyond Born - Oppenheimer equation for the excited states of Sodium trimer,
A. K. Paul, B. Sarkar and S. Adhikari
Chapter in Recent Advances in Spectroscopy, Pub: Springer Verlag, Eds: Chaudhuri, R.K.; Mekkaden, M.V.; Raveendran, A.V.; Satya Narayanan, A. (2010) p. 63.

9. A treatise on the interaction of molecular system with short - pulse highly - intense

external fields,
A. K. Paul, S. Adhikari and M. Baer,
Phys. Rep. **496**, 79 (2010).
Impact Factor: **22.910**

10. A quantum-classical simulation of the nuclear dynamics in NO_2^- and $C_6H_6^+$with realistic model Hamiltonian,
S. Sardar, **A. K. Paul** and S. Adhikari,
J. Chem. Sci. **122**, 491 (2010).
Impact Factor: **1.224**

11. A classical trajectory driven nuclear dynamics by a parallelized quantum classical approach to a realistic model Hamiltonian of benzene radical cation,
S. Sardar, **A. K. Paul**, R. Sharma, and S. Adhikari,
Int. J. Quan. Chem. **111**, 2741 (2011).
Impact Factor: **1.166**

12. Conical intersections in $2^2E'$ states of Na_3 cluster,
A. K. Paul, S. Ray, D. Mukhopadhyay and S. Adhikari,
Chem. Phys. Letts. **508**, 300 (2011).
Impact Factor: **1.991**

13. Ab initio calculations on the excited states of Na3 cluster to explore beyond Born – Oppenheimer theories: Adiabatic to diabatic PESs and nuclear dynamics,
A. K. Paul, S. Ray, D. Mukhopadhyay and S. Adhikari,
J. Chem. Phys. **135**, 034107 (2011).
Impact Factor: **3.122**

14. Adiabatic to Diabatic transformation and nuclear dynamics on diabatic Hamiltonian constructed by using ab initio potential energy surfaces and non - adiabatic coupling terms for excited states of Sodium trimer,
A. K. Paul, S. Ray and S. Adhikari
Chapter in Proceedings of JT 2010, Pub: Springer, Eds: M. Atanasom and C. Dual
p. 281 (2012).

Post Ph.D. Publications

15. The molecular symmetry adapted non - adiabatic coupling terms and diabatic Hamiltonian matrix,
S. Mukherjee, S. Bandyopadhyay, **A. K. Paul** and S. Adhikari
Journal of Physics: Conference Series **428**, 012008 (2013)

16. Conical intersections between X^2A_1 and A^2B_2 electronic states of NO_2
S. Sardar, S. Mukherjee, **A. K. Paul**, and S. Adhikari,
Chem. Phys. **416**, 11 (2013).
Impact Factor: **2.028**

17. Construction of Diabatic Hamiltonian Matrix from *ab Initio* Calculated Molecular Symmetry Adapted Nonadiabatic Coupling Terms and Nuclear Dynamics for the Excited States of

Na_3 Cluster
S. Mukherjee, S. Bandyopadhyay, **A. K. Paul** and S. Adhikari
J. Phys. Chem. A **117**, 3475 (2013).
Impact Factor: **2.883**

18. Models for Intrinsic Non-RRKM Dynamics. Decomposition of the S_N2 Intermediate Cl^-–CH_3Br
M. Paranjothy, R. Sun, **A. K. Paul**, and W. L. Hase
Z. Phys. Chem. **227**, 1361 (2013).
Impact Factor: **1.178**

19. Computation of Intrinsic RRKM and Non-RRKM Unimolecular Rate Constants.
A. K. Paul, S. Kolakkandy, S. Pratihar, and W. L. Hase
Chapter 20 of the book titled: "*Reaction Rate Constant Computation: Theory and Computation*", Pub: Royal Society of Chemistry, Eds: Keli Han, and Tianshu Chu, p. 494 (2013).

20. A Unified Model for Simulating Liquid and Gas Phase Intermolecular Energy Transfer. N_2 + C_6F_6 Collisions
A. K. Paul, S. C. Kohale, S. Pratihar, R. Sun, S. W. North, and W. L. Hase
J. Chem Phys. **140** 194103 (2014).
Impact Factor: **3.122**

21. Energy and Temperature Dependent Dissociation of the $Na^+(Benzene)_{1,2}$ Complexes
S. Kolakkandy, **A. K. Paul**, S. Pratihar, G. Barnes, and W. L. Hase
J. Chem. Phys. **142**, 044306 (2015).
Impact Factor: **3.122**

22. Potential Energy Surfaces for the $HBr^+ + CO_2 \rightarrow Br + HOCO^+$ Reaction in the HBr^+ $^2\Pi_{3/2}$ and $^2\Pi_{1/2}$ Spin-Orbit States
R. Sun, G. Granucci, **A. K. Paul**, M. Siebert, H. Liang, G. Cheong, W. L. Hase, and M. Persico
J. Chem. Phys. **142**, 104302 (2015).
Impact Factor: **3.122**

23. Bath Model for N_2 + C_6F_6 Gas-Phase Collision: Detail of Intermolecular Energy Transfer Dynamics
A. K. Paul, S. Kohale and W. L. Hase
J. Phys. Chem. C, **119**, 14683 (2015).
Impact Factor: **4.835**

24. Dynamics of Na^+(Benzene) + Benzene Association and Ensuing $Na^+(Benzene)_2$* Dissociation
A. K. Paul, S. Kolakkandy, and W. L. Hase
J. Phys. Chem. A, **119**, 7894 (2015).
Impact Factor: **2.883**

25. Chemical Dynamics Simulation of Benzene Dimer Dissociation
X. Ma, **A. K. Paul**, W. L. Hase
J Phys. Chem. A. **119**, 6631 (2015).
Impact Factor: **2.883**

26. A Zero Point Energy Constraint for Unimolecular Dissociation Reactions. Giving Trajectories Multiple Chances to Dissociate Correctly
A. K. Paul and W. L. Hase
J Phys. Chem. A. **120**, 372 (2016)
Impact Factor: **2.883**

27. Chemical Dynamics Simulations of Intermolecular Energy Transfer: Azulene + N_2 Collisions
H. Kim, **A. K. Paul**, S. Pratihar, and W. L. Hase
J. Phys. Chem. A **120**, 5187-5196 (2016)
Impact Factor: **2.883**

Publications NIT Meghalaya Affiliation

28. Collisional Intermolecular Energy Transfer From a N_2 Bath at Room Temperature to a Vibrationlly "Cold" C_6F_6 Molecule Using Chemical Dynamics Simulations.
A. K. Paul, D. Donzis, and W. L. Hase
J. Phys. Chem. A, **121**, 4049-4057 (2017).

29. Plastically bendable crystals of probenecid and its cocrystal with 4,4′ -Bipyridine.
N. K. Nath*, M. Hazarika, P. Gupta, N. R. Ray, **A. K. Paul***, E. Nauha*
J. Mol. Struc. **1160**, 20-25 (2018).

30. PSO Method for Fitting an Analytic Potential Energy Function. Application to $I^-(H_2O)$
H. N. Bhandari, X. Ma, **A. K. Paul**, P. Smith, W. L. Hase
J. Chem. Theo. Comput. **14**, 1321-1332 (2018).

31. Non-statistical intermolecular energy transfer from vibrationally excited benzene in a mixed nitrogen-benzene bath
A. K. Paul, N. A. West, J. D. Winner, R. D. W. Bowersox, S. W. North, and W. L.Hase
J. Chem. Phys. **149**, 134101 (2018)

32. A better understanding of the unimolecular dissociation of weakly bound aromatic complexes: A study on C_6H_6-C_6F_6 and comparison with C_6H_6-C_6H_6.
H. Mahanta, D. Baishya, S. S. Ahamed, **A. K. Paul***
J. Phys. Chem. A 123, 2517-2526 (2019)

33. Chemical Dynamics Simulations on Association and Ensuing Dissociation of Benzene-Hexafluorobenzene Molecular System.
H. Mahanta, D. Baishya, S. S. Ahamed, **A. K. Paul***
J. Phys. Chem. A 123, 5019-5026 (**2019**)

34. Unimolecular dissociation of C_6H_6-C_6F_6 complex in N_2 bath and comparison with gas phase dynamics
S.S. Ahamed, H. Mahanta, **A. K. Paul***
Chem. Phys. Letts. 730, 630-633 (2019).

35. A Competition Between Dissociation Pathway and Energy Transfer Pathway: Unimolecular Dissociation of Benzene-Hexafluorobenzene Complex in Nitrogen Bath
S.S. Ahamed, H. Mahanta, **A. K. Paul***
J. Phys. Chem. A, 123, 10663-10675 (2019)

36. Mode-to-Mode Collision Energy Transfer from Vibrationally Excited C_6F_6 to NO/N_2 Mixed Bath with the Development of New Potential Energy Functions
S. S. Ahamed, P. Kumar, H. Kalita, **A. K. Paul***
Chem. Select, **5**, 10475-10487 (2020)

37. Unimolecular Dissociation Dynamics of C_6H_6-C_6Cl_6 Complex and The Effect of Anharmonicity
H. Mahanta, Sumadevi N., R. Mishra, **A. K. Paul***
Int. J. Mass. Spectrometry. **456**, 116392 (2020)

38. Comparison of Intermolecular Energy Transfer from Vibrationally Excited Benzene in Mixed Nitrogen-Benzene Baths at 140 and 300 K
S. S. Ahamed, H. Kim, **A. K. Paul***, N. A. West, J. D. Winner, D. A. Donzis, S. W. North, and W. L. Hase
J. Chem. Phys. **153**, 144116 (2020)

39. A Photochemical Intramolecular C-N Coupling Towards the Synthesis of Benzimidazole-Fused Phenanthridines.
Shyamal Kanti Bera, Palash J. Boruah, Shraddha Saraswati Parida, **Amit K. Paul*** and Prasenjit Mal*
J. Org. Chem. 86, 9587–9602 (2021)

40. Unimolecular Dissociation of C_6H_6-C_6Cl_6 Complex and Effect of Mode-Mode Coupling
Himashree Mahanta and **Amit K. Paul***
J. Phys. Chem. A 2021, 125, 27, 5870–5877

41. Dynamical Behavior of Aromatic Trimer Complexes in Unimolecular Dissociation Reaction at High Temperatures. Case Studies on C_6H_6-C_6F_6-C_6H_6 and C_6H_6-trimer Complexes
Himashree Mahanta and **Amit K. Paul***
J. Phys. Chem. A 126, 259–271 (2021)

42. Oxidized Charcoal-Supported Thiol-Protected Palladium Nanoparticles for Cross Dehydrogenative Coupling of Heteroarenes.
S. Kumar, S. Kumari, S. Singh, P. J. Boruah, **A. K. Paul**, P. Roy, and H. Joshi
ACS Appl. Nano Mater. 5, 2644–2654 (2022).

43. An Advanced Bath Model to Simulate Association Followed by Ensuing Dissociation Dynamics of Benzene + Benzene System: A Comparative Study of Gas and Condensed Phase Results.
Sk. Samir Ahamed, Himashree Mahanta, and **Amit K. Paul***
Phys. Chem. Chem. Phys. 24, 23825 (2022)

44. Post Transition State Direct Dynamics Simulations on the Ozonolysis of Catechol
A. Agarwal, P. J. Boruah, B. Sarkar, and **A. K. Paul***

J. Phys. Chem. A 126, 5314 (2022).

45. Visible Light-Induced Ternary Electron Donor-Acceptor Enabled Synthesis of 2-(2-Hydrazinyl) thiazole Derivatives and The Assessment of Their Antioxidant and Antidiabetic Therapeutic Potential
Sovan Dey, Arindam Das, Ram Naresh Yadav, Palash Jyoti Boruah, Prerana Bakli, Tania Baishya, Koushik Sarkar, Anup Barman, Ranabir Sahu, Biplab Maji, **A. K. Paul**, Md. Firoj Hossain
Org. Biomol. Chem., 21, 1771-1779 (2023).

46. An Expeditious One-Pot Two-Component Synthesis of Quinoxaline Derivatives in Natural Deep Eutectic Solvents (NADESs)
Arindam Das, Sovan Dey, Ram Naresh Yadav, Palash Jyoti Boruah, Prerana Bakli, Sourav Sarkar, Partha Mahata, **A. K. Paul**, Md. Firoj Hossain
Chem. Select. 8, e202204651 (2023)

47. Details of Ozonolysis of Catechol at High Temperature and Product Energy Distribution
Ankita Agarwal, **A. K. Paul***
J. Chem. Sci. 135, 33 (2023).

48. Unimolecular Dissociation of C_6H_6-C_6H_5Cl, C_6H_6-$C_6H_3Cl_3$, and C_6H_6-C_6Cl_6 Complexes using Machine Learning Approach
Basudha Deb, S R Ngamwal Anal, Himashree Mahanta, Yogita, and **A. K. Paul***
J. Chem. Phys. 158, 194104 (2023).

49. Post Transition State Direct Dynamics Simulations on the Ozonolysis of Catechol in N_2 bath and comparison with gas phase dynamics
Ankita Agarwal, Shrutimala Baruah, Samir Ahmed, Palash Boruah, and **A. K. Paul***
J. Phys. Chem. A, 127, 6804–6815 (2023).

50. On the Intramolecular Vibrational Energy Redistribution Dynamics of Aromatic Complexes: A Comparative Study on C_6H_6 - C_6H_5Cl, C_6H_6 - $C_6H_3Cl_3$, C_6H_6 - C_6Cl_6 and C_6H_6 - C_6H_5F, C_6H_6 - $C_6H_3F_3$, C_6H_6 - C_6F_6
B. Deb, H. Mahanta, N. P. Baruah, M. Khardewsaw, and **A. K. Paul***
J. Chem. Phys. **160**, 024307 (2024).

51. Details of Exit Channel Dynamics of the Ozonolysis of Catechol in Condensed Phase: Product Channels and Product Energy Partitioning
A. Agarwal and **A. K. Paul***
Chem. Phys. Impact, **8**, 100440 (2024).

52. A Theoretical Investigation to Understand the Difference in Reactivities of Secondary and Tertiary Propargylic Alcohols with 1,3,5-Trimethoxybenzene in Presence of Brnøsted Acid
P. J. Boruah, M. Debnath, A. Agarwal, G. Kalita, P. N. Chatterjee*, and **A. K. Paul***
Int. J. Chem. Kinet. 2024;1-12. https://doi.org/10.1002/kin.21714.

53. Unleashing Naphthopyranopyrimidine's Anticancer Potential: A Deep Eutectic Solvent (DES) Study

A. Das, S. Dey, R. N. Yadav, P. Dutta, S. Dhiman, P. Boruah, K. Sarkar, A. Sahu, A. Jana, A. K. Paul, and M. F. Hossain,
New Journal of Chemistry, **48**, 7566 (2024)

54. A Detailed Theoretical Investigation on Intramolecular Charge Transfer Mechanism of Primary, Secondary, and Tertiary p-amino Substituted Benzaldehyde,
P. J. Boruah, Venkatesh N, A. Samanta*, **A. K. Paul***
Chem. Phys. Impact **8**, 100538 (2024). (Special Issue: Recent Trends of Physical Chemistry in India)

Publications with Bose Institute Affiliation

55. Electron donor–acceptor complex enabled photocascade strategy for the synthesis of trans-dihydrofuro[3,2-c]chromen-4-one scaffolds via radical conjugate addition of pyridinium ylide
S. Dey, A. Das, R. N. Yadav, P. J. Boruah, K. Sarkar, **A. K. Paul**, and Md. F. Hossain,
Chem. Commun., 60, 14384-14387 (2024)

56. Exploring Anticancer Potential of Furopyrano[3,4-b]indole via Graphene Oxide-Catalyzed Aqueous Synthesis
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Important Administrative Responsibilities Performed at NIT Meghalaya

Sl. No.	Post	Duration	Responsibilities
1	Academic Coordinator of B.Tech. First Year Students	Sept. 2016 – Sept. 2017	Since in B.Tech. First year courses are common, instead of put them under respective department, they are assigned a general coordinator
2	Member, Sports Committee	Sept. 2016 – June 2019	To take care of various sports activities
3	Member, NSS committee	January 2017 – till date	To take care of NSS activities of the Institute
4	Convenor, Convocation	From 2017 till 2021	Invitation and Reception
5.	Coordinator, B. Tech. and M.Sc. Admission	July 2017	To monitor B.Tech. and M.Sc. admission of the Institute
6	Faculty-in-charge, Cultural committee	July 2017 – June 2018	Responsibility of all kinds of cultural activities of the Institute
7	Chairman, Institute Routine committee	July 2017 – June 2019	To prepare general routine for all courses of the entire Institute
8	Vice Chairman, Institute Day celebration	2018, 2019, 2022	To monitor the progress and smooth conduct of the foundation day function
9	Hostel Warden	July 2018 – June 2021	Warden of two hostels (PhD from 2018-2020 and (B.Tech. 2nd year from 2020-21)
10	Chairman, On-campus business committee	July 2019-June 2021	To take care of all kinds of on campus business of the Institute
11	Member, Library	July 2019 – May	Departmental representative of the committee

	committee	2024	
12	President, Student Activity Centre	July 2021 – July 2023	To take care of all cultural, technical, and sports activities of the Institute
13	Professor-in-charge, Institute Transit house & Guesthouse	February 2023 – July 2023	To take care of the activity and maintenance of the Transit house and guesthouse.
14	Head of the Department, Department of Chemistry, NIT Meghalaya	July 2023 – May 2024	To work for the betterment of the Department and place the departmental stand points to the Institute.

Important Administrative Responsibilities Performed at Bose Institute

Sl. No.	Post	Duration	Responsibilities
1	Convenor of Software Procurement Committee	Jan. 2025 till date	To enquire the requirement of software in various labs of the Institute and to expedite the procurement processes
2	Coordinator of Ph.D. admission to DCS	2024 and 2025	To carry out the underlying processes of the interview till the selection of the candidates in the department of Chemical Sciences
3	Coordinator of Ph.D. counselling	2025	To conduct the counseling of the selected candidates for the final allotment of labs
4	Member of Purchase and Payment monitoring committee	2025 – till date	To monitor the ongoing purchase and payment processes of the Bose Institute
5.	Member of Annual Report Committee	2025 – till date	To help compiling and finalize the annual report draft of the Bose Institute