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
1	reducity 2015 – Julie 2010	Texas Tech University
2	June 2016 – November 2017	Assistant Professor (consolidated pay),
<u> </u>	June 2010 – November 2017	NIT Meghalaya
3	November 2017 September 2010 Assistant Professor Gra	Assistant Professor Grade II, NIT
3	November 2017 – September 2019	Meghalaya
4	September 2019 – December 2023	Assistant Professor Grade I, NIT
4	September 2019 – December 2023	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.
- (1) 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 to 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 systems, reaction dynamics
- (b) Condensed phase calculation for various solute solvent interaction, namely, C₆F₆, C₆H₆, and C₁₀H₈, in interaction with the solvent like N₂, NO, H₂O etc.
- (c) Developing package for electronic non-adiabatic dynamics: With semiclassical surface hopping algorithm
- (d) Developing simulation package with Machine Learning algorithms

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

	Chemical Reactions and the Effect of Solvation			August 2022
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	То	Courses Taught	M.Sc. Project	Ph.D.
			guided	guided
Aug.	Till Date	1. Quantum Mechanics,	16 (completed)	2
2016		2. Chemical Kinetics,	2 (ongoing)	6(ongoing)
		3. Molecular Spectroscopy,		
		4. Computational Chemistry,		
		5. Group Theory		
		6. Environmental Science		

Ph.D. Degree Awarded:

Sl.	Name	Date of	Title of the Thesis	Current Position
No.		Degree		
1	Dr. Himashree	23/05/2022	The Understanding of the Intramolecular	Assistant Professor,
	Mahanta		Interactions in Aromatic	Assam Kaziranga
			Complexes through Computational	University
			Investigations of Unimolecular	
			Dissociation and Association Reactions	
2	Dr. Sk. Samir	05/09/2022	Molecular Dynamics Simulation on	Post-doctoral Fellow,
	Ahamed		Energy Transfer and Chemical Reactions	SNBNCBS, Kolkata
			in Single/Mixed Bath Molecular Systems	
3	Dr. Ankita Agarwal	21/05/2024	Post-Transition State Dynamics on	
			Ozonolysis of Catechol in Gas and	
			Condensed Phase	

Complete List of Publications

I. Published Articles:

- 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 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 H₂⁺ 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 Na₃ cluster,
- A. K. Paul, S. Sardar, B. Sarkar and S. Adhikari,

J. Chem. Phys. 131, 124312 (2009).

Impact Factor: 3.122

6. H₂⁺ 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 NO₂⁻ and C₆H₆⁺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 2²E' states of Na₃ 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 X²A₁ and A²B₂ electronic states of NO₂
- 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 Na₃ 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⁻– CH₃Br
- 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. N₂ + C₆F₆ 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 From NIT Meghalaya

28. Collisional Intermolecular Energy Transfer From a N₂ Bath at Room Temperature to a

Vibrationlly "Cold" C₆F₆ 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 (H₂O)
- 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 C₆F₆ to

NO/N₂ 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 C₆H₆-C₆Cl₆ 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 C₆H₆-C₆Cl₆ 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 C₆H₆-C₆H₅Cl, C₆H₆-C₆H₃Cl₃, and C₆H₆-C₆Cl₆ 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 N₂ 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)

Conferences, Seminars, Workshops, Organized

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

Invited Talks

- 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

- 9. Invited talk in the workshop on High Performance Computing and it's Multidiciplinary Applications, NIT Meghalaya, August 22 27, 2022
- 10. Invited Young Scientist Lecture in ETCS 2023, NEHU, 2 4 March 2023
- 11. Invited Talk in MS-TPCCP at IIT-B, 29-30 July 2023
- 12. Resource person talk at Refresher Course in Chemistry at NEHU, 5th August 2023
- 13. Invited talk at MS-PCCP in IIT Bombay, July 29-30, 2023.
- 14. Invited talk at IC-SDSS 2023, IACS, October 5-8, 2023.
- 15. Invited talk at QSCP, Jaipur, 14-20 October, 2023
- 16. Invited talk at SoPhyC Inaugural conference, IIT Kanpur, 29 31 October 2023
- 17. Invited hot topic talk at iCOMET, Jaipur, November 12 16, 2023
- 18. Invited Talk at SDMC 2024, Kaziranga, Feb. 22-25, 2024
- 19. Invited talk at RTCST 2024, IIT Patna, March 1-2, 2024
- 20. Invited talk at Machine Learning workshop at NIT Durgapur, March 3, 2024

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. 2 nd 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 committee	July 2019 – May 2024	Departmental representative of the committee
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.