Dr. Tapta Kanchan Roy

Assistant Professor (from August, 2016)
Department of Chemistry & Chemical Sciences
Central University of Jammu
Rahya-Suchani (Bagla), District-Samba
Jammu-181143, (J&K) India
Phone No: 09831957705
e-mail: taptakanchan@gmail.com , tapta.che@cujammu.ac.in

Group Web Site: https://sites.google.com/view/theochem-cuj/home

Major area of interest: **Theoretical and Computational Chemistry**

Specialization:

- Anharmonic vibrational spectroscopy, Potential energy surfaces, Many-body theory, Quantum statistical mechanics

Positions

January, 2015- May, 2016	:	**Assistant Professor** Department of Chemistry Central University of Rajasthan, Rajasthan
August, 2012 - December, 2014	:	**PBC Post-doctoral Research Fellow** With Prof. R. Benny Gerber, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Israel
August, 2011 – June 2012	:	**Post-doctoral Research Fellow** With Dr. Rochus Schmid, Computational Material Chemistry, Ruhr University, Bochum, Germany
March, 2011 – May, 2011	:	**Research Associate** With Prof. S. Mahapatra, School of Chemistry, University of Hyderabad, Hyderabad, India
August, 2005 – Feb, 2011	:	**Doctoral Research Fellow** With Prof. M. Durga Prasad, School of Chemistry, University of Hyderabad, Hyderabad, India

Academic Background

PhD (Chemistry), 2010	:	School of Chemistry, University of Hyderabad, India
PhD Thesis Title	:	Development of Separable Ansatze for the Description of Molecular Vibrations
MSc (Chemistry), 2004	:	Banaras Hindu University, Varanasi, India
BSc (Chemistry), 2002	:	Presidency College, University of Calcutta, Kolkata, India

Current research interests:

- Development of new formalism for anharmonic vibrational spectroscopy
- Machine Learning algorithm for potential energy surfaces
- Many-body theory
- Quantum statistical mechanics
- Development of computational chemistry software and massively parallel algorithm

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Software Development:

Developer of GAMESS computational chemistry software and other in-house software

Previous Research

1) Development of algorithm and investigation of anharmonic IR spectra of large biological molecules like peptides, ploy-saccharides and proteins.
2) Atomistic modeling and simulations of hybrid material systems: a systematic development and parameterization of polarizable and reactive force fields.
3) Investigation of anharmonic molecular vibrations using vibrational self-consistent field (VCSF) and effective harmonic oscillator (EHO) theory to determine different physical and chemical properties of molecular systems, using quantum mechanical ansatze and thermal density matrices.
4) Investigation of structure, reactivity and stability of different high energy density molecules and conformational analysis, and its application to high energetic polymer chemistry
5) Investigation of reaction mechanism for complex bio-molecular reactions and proton transfer.

Projects:

Ongoing

1. SERB-MATRICS, 2022-2025 (6.6 lacs)
2. SERB-CRG, 2023-2026 (~40 lacs)

Completed

1. DST-EMR grant, 2017-2020 (55.1 lakh)
2. UGC-startup grant, 2017-2019 (10 lakh)
3. University startup grant from CU Jammu (2 lakhs)

PhD Guidance: Completed: 1, Ongoing: 2
MSc/BSc Project guidance : Completed: 25, Ongoing: 4

List of Publications

Total no. of publications (Peer reviewed, International) = 45
Book Chapter (International) = 1
***h*-index = 21,** ***i*-10-index = 25** (up to December 2023)

2023

45. Accuracy of Different Electronic Basis Set Families for Anharmonic Molecular Vibrations: A Comprehensive Benchmark Study
D. Sharma and **T. K. Roy***
J. Phys. Chem. A, 127, 7132–7147, (2023), ISSN: 1520-5215,
https://doi.org/10.1021/acs.jpca.3c02874

44. The importance of electron correlations on vibrational anharmonicities and potentialenergy surfaces
A. Fayaz, S. Banik* and **T. K. Roy***
Comput. Theor. Chem., 122, 114059, **(**2023), ISSN: 2210-271X,
https://doi.org/10.1016/j.comptc.2023.114059

43. Sulfonated Polybenzimidazole as a PEM in a Microbial Fuel Cell: An Efficient Strategy forGreen Energy Generation and Wastewater Cleaning
S. Subhadarshini, J. S. Sravan, O. Sarkar, S. V. Mohan, **T. K. Roy** and T. Jana
ACS Appl. Energy Mater., 6, 1422–1438, (2023) ISSN: 2574-0962,
https://doi.org/10.1021/acsaem.2c03238

42. Exploring the stereochemistry ofIn(III)-A3B-type porphyrins axiallyligated with p-PDA: synthesis,electronic properties and DFTcalculations
D. Sharma, S. Kundan, A. Fayaz and **T. K. Roy**
J. Coord. Chem. (2022)
https://doi.org/10.1080/00958972.2023.2276051

2022

41. Effects of non-local exchange functionals in the density functional theories forthe description of molecular vibrations
A. Fayaz, **T. K. Roy,*** and S.Banik,*
J. Chem Sc., 134, 67, (2022), ISSN: 0973-7103
https://doi.org/10.1007/s12039-022-02061-1

40. Performance of Vibrational Self-Consistent Field Theory for Accurate Potential Energy Surfaces: Fundamentals, Excited States, and Intensities.
T. K. Roy*
J. Phys. Chem. A, 126, 608–622, (2022), ISSN: 1520-5215
https://doi.org/10.1021/acs.jpca.1c09989

39. Halloysite nanotubes functionalized sulfonic acid: synthesis, spectroscopic characterization, computational studies and application for the synthesis of 1,4-dihydropyridines
P. Gupta,* N. Prakash, Y. Ramawat, P. Rajput, A. Fayaz, **T. K. Roy**
Lett. Org.Chem., 19, 19, (2022), ISSN: 1875 6255,
https://doi.org/10.2174/1570178618666210302160130

38. Light-induced energy and electron transfer occurring in tandem in tetra (bis(4′-tert-butylbiphenyl-4-yl)aniline)-zinc(II) porphyrin-fullerene supramolecular conjugates
G. Suneel, K. Jain, B. Aajaiah, H. Mitra, R. A. Ramnagar, S. Bandi, V. Chuncha, **T. K. Roy**, L. Giribabu, R. Chitta
Journal of Porphyrins and Phthalocyanines, 26, 872-883, (2022), ISSN: 1099-1409
https://doi.org/10.1142/S1088424622500705

2021

37. Porphyrin bearing phenothiazine pincers as hosts for fullerene binding via concave–convex complementarily: synthesis and complexation study
K. Jain, N.Duvva, **T. K. Roy**,* L.Giribabu* and R. Chitta*
New J. Chem., 45, 19691–19703, (2021), ISSN: 1144-0546,
https://doi.org/10.1039/D1NJ03727G

2020

36. Rhodium(III)-Catalyzed Annulation of 2-Arylimidazo[1,2-a]pyridines with Maleimides: Synthesis of 1H-Benzo[e]pyrido[1′,2′:1,2]imidazo[4,5-g]isoindole -1,3(2H)-Diones and their Photophysical Studies
V. N. Shinde, **T. K. Roy**, S. Jaspal, D. S. Nipate, N. Meena, K. Rangan, D. Kumar, A. Kumar
Adv. Synth. Catal., 362, 5751-5764, (2020), ISSN 1615-4169,
https://doi.org/10.1002/adsc.202000960

35. Comprehensive Benchmark Results to the Accuracy of Basis Sets for the Anharmonic Molecular Vibrations
H. Mitra and **T. K. Roy***
J. Phys. Chem. A, 124, 44, 9203–9221, (2020), ISSN: 1520-5215,
https://doi.org/10.1021/acs.jpca.0c06634

34. Dual Basis Approach for Ab Initio Anharmonic Calculations of Vibrational Spectroscopy: Application to Micro-Solvated Biomolecules
T. K. Roy* and R. B. Gerber.
J. Chem. Theory Comput. 16, 11, 7005–7016, (2020), ISSN: 1549-9618, https://doi.org/10.1021/acs.jctc.0c00725

33. Comprehensive Analysis of Band Gap and Nanotwinning in $Cd_{1-x}Mg_xS$ QDs
T. Kalsi, H. Mitra, **T. K. Roy**, S. K. Godara and P. Kumar
Cryst. Growth Des. 20, 10, 6699–6706, (2020), ISSN**:** 1528-7483,
https://doi.org/10.1021/acs.cgd.0c00851

32. On the Proton Shuttle Motion in Protonated Acetylene: AnElectronic Structure Perspective
S. Banik, A. K. Sansi, S. Nandan. and **T. K. Roy***
ChemistrySelect, *5*, 9288 –9295, **(**2020) ISSN:2365-6549,
https://doi.org/10.1002/slct.202002524

31. Dinuclear gold(I)-N-heterocyclic carbene complexes: Synthesis, characterization, and catalytic application for hydrohydrazidation of terminal alkynes
S. Yadav, S. Ray, A Singh, S. M. Mobin, **T. K. Roy***, C. Dash.
Appl. Organomet. Chem., 34, e5942, (2020) ISSN**:** 1099-0739,
https://doi.org/10.1002/aoc.5942

30. Conjugated Small Organic Molecules: Synthesis and Characterization of 4-Arylpyrazole-decorated Dibenzothiophenes
S. Panda, R. S. Jat, A. Fayaz, J. Saha, R. Thirumoorthi, **T. K. Roy** and M. Bhanuchandra
New J. Chem., 44,8944-8951, (2020) ISSN: 1144-0546,
https://doi.org/10.1039/D0NJ01887B

29. Designed Synthesis, Characterization and Evaluation of Anticancer Activity of Water-Soluble Half-sandwich Ruthenium (II)Arene Halido Complexes
T. A. Khan, K. Bhar, R. Thirumoorthi, **T. K. Roy*** and A. K. Sharma*
New J. Chem., 44, 239-257 (2020), ISSN: 1144-0546,
https://doi.org/10.1039/C9NJ03663F

2019

28. Novel axially ligated complexes of Zn(II)porphyrin: spectroscopic, computational, and antibiological characterization
S. Kundan, G. D.Bajju, D. Gupta, **T. K. Roy**
Russian J. Inorg. Chem.,*64*, 1379–1395 (2019),ISSN: 1531-8613, https://doi.org/10.1134/S003602361911010X

2018

27. Intrinsic Structure of Pentapeptide Leu-enkephalin: Geometry Optimization and Validation by Comparison of VSCF-PT2 Calculations with Cold Ion Spectroscopy
T. K. Roy, V. Kopysov, A. Pereverzev, J. Šebek,R. B. Gerber,* and O. V. Boyarkin*
Phys. Chem. Chem. Phys. 20, 24894-24901 (2018). ISSN: 1463-9076, https://doi.org/10.1039/C8CP03989E

26. Phosphine-Free Bis(Pyrrolyl)pyridine based NNN-pincer Palladium(II) Complexes as Efficient Catalysts for Suzuki-Miyaura Cross-Coupling Reactions of Aryl Bromides in Aqueous Medium
S. Yadav, A. Singh,N. Rashid,M. Ghotia, **T. K. Roy**, P. P. Ingole,S. Ray, M. M. Shaikhand C. Dash
ChemistrySelect. (2018), 3, 9469-9475, ISSN**:** 2365-6549, https://doi.org/10.1002/slct.201801647

25. Hypochlorite-Mediated Modulation of Photoinduced Electron Transfer in a Phenothiazine-Boron dipyrromethene Electron Donor-Acceptor Dyad: A Highly Water Soluble "Turn-On" Fluorescent Probe for Hypochlorite
D. Soni, N. Duvva, D. Badgurjar, **T. K. Roy,** S. Nimesh, G. Arya. L. Giribabu, R. Chitta
Chem. Asian. J., 13, 1594-1608, (2018), ISSN**:** 1861-4728, https://doi.org/10.1002/asia.201800349

24. Synthesis of Spirooxindoles through Cyclocondensation of Isatin and Cyclic 1,3-Diones
R. Joshi, A. Kumawat, S. Singh, T. K. Roy, R. T. Pardasani,
J. Heterocycl. Chem., 55, 1783-1790 (2018), ISSN: 1943-5193, https://doi.org/10.1002/jhet.3217

23. Catalyst-Controlled Structural Divergence: Selective Intramolecular 7-*endo-dig* and 6-*exo-dig* Post-Ugi Cyclization for the Synthesis of Benzoxazepinones and Benzoxazinones
K. Singh, B. K. Malviya**, T. K. Roy**, V. S. Mithu, V. K. Bhardwaj, V. P. Verma, S. S. Chimni, S. Sharma
J. Org. Chem, 83, 1, 57-68, (2018), ISSN: 00223263. https://doi.org/10.1021/acs.joc.7b02123

2017

22. Azo-dyes based small bifunctional molecules for metal chelation and controlling amyloid formation
M. Rana, H. J. Cho, **T. K. Roy** , L. M. Mirica, A. K. Sharma*,
Inorganica Chim. Acta, 471, 419-429, (2017), ISSN: 0020-1693, https://doi.org/10.1016/j.ica.2017.11.029

21. Synthesis of Diverse Nitrogen Heterocycles via Palladium-Catalyzed Tandem Azide–Isocyanide Cross-Coupling/Cyclization: Mechanistic Insight using Experimental and Theoretical Studies

J. Ansari, R. S. Pathare, A. K. Maurya, V. K. Agnihotri, S. Khan, **T. K Roy,*** D. M. Sawant,*
and R. T. Pardasani*
Adv. Synth. Catal., 360, 2, 290-297, (2017), ISSN: 1615-4150,
https://doi.org/10.1002/adsc.201700928

20. A Decapeptide Hydrated by Two Waters: Conformers Determined by Theory and Validated by Cold Ion Spectroscopy
T. K. Roy, N. S. Nagornova, O. V. Boyarkin and R. B. Gerber
J. Phys. Chem. A.121, 48, 9401-9408, (2017) ISSN: 1520-5215,
https://doi.org/10.1021/acs.jpca.7b10357

19. Hypochlorite promoted inhibition of photo-induced electron transfer in phenothiazine-borondipyrromethene donor-acceptor dyad: A cost-effective and metal-free "turn-on" fluorescent chemosensor for hypochlorite
D. Soni, S. Gangada, N. Duvva, **T. K. Roy**, S. Nimesh, G. Arya, G. Lingamallu and R. Chitta
New J. Chem., 41, 5322-5333, (2017), ISSN: 1144-0546,
https://doi.org/10.1039/C7NJ00516D

2016

18. A catalyst-free one-pot multicomponent synthesis of spirobenzimidazoquinazolinones via Knoevenagel-Michael-Imine pathway: A microwave assisted approach
P. Maloo, **T. K. Roy**, D. Sawant, R. T. Pardasani and M. M. Salunkhe.
RSC Advances, 6, 41897 (2016). ISSN: 1523-7060,
https://doi.org/10.1039/C6RA05322J

17. Ruthenium catalyzed intramolecular C-S coupling reactions: Synthetic scope and mechanistic insights
S. Sharma, R. S. Pathare, A. K. Maurya, K. Gopal, **T. K. Roy**, D. M. Sawantand R. T. Pardasani
Organic Letters, 18, 365, (2016), ISSN: 1523-7060,
https://doi.org/10.1021/acs.orglett.5b03185

16. First-Principles Anharmonic Quantum Calculations for Peptides Spectroscopy: VSCF Calculations and Comparison with Experiment
T. K. Roy, R. Sharma and R. B. Gerber
Phys. Chem. Chem. Phys. 18, 1607 (2016). ISSN: 1463-9076,
https://doi.org/10.1039/C5CP05979H

2015

15. Mechanistic Studies of Malonic Acid-Mediated in situ Acylation
K. Chandra, J. N. Naoum, **T. K. Roy**, C. Gilon, R. B. Gerber and A. Friedler
Biopolymers, 104, 495 (2015). ISSN: 1097- 0282,
https://doi.org/10.1002/bip.22654

14. Conformational Structures of a Decapeptide Validated by First-Principles Calculations and Cold Ion Spectroscopy
T. K. Roy, V. Kopysov, N. S. Nagornova, T. R. Rizzo, O. V. Boyarkin and R. B. Gerber
ChemPhysChem, 16, 1374 (2015). ISSN: 1439- 7641,
https://doi.org/10.1002/cphc.201500085

2014

13. Approximate First Principles Anharmonic Calculations of Polyatomic Spectra using MP2 and B3LYP Potentials: Comparisons with Experiment
T. K. Roy, T. Carrington. Jr. and R. B. Gerber
J. Phys. Chem. A, 118, 6730, (2014). ISSN: 1520-5215,
https://doi.org/10.1021/jp5060155

12. A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage
K. Chandra, **T. K. Roy**, D. E. Shalev, A. Loyter,C. Gilon R. B. Garber, A. Friedler
Angew. Chem. Int. Ed., 53, 9450, (2014). ISSN: 1521- 3773,
https://doi.org/10.1002/ange.201402789

11. A Highly Efficient *in situ* Acetylation Approach for Diverse Polyfunctionalized Complex Network
K. Chandra, **T. K. Roy**, J. Naoum, C. Gilon, R. B. Garber and A. Friedler
Org. Biomol. Chem. 12, 1879 (2014). ISSN: 1477-0520,
https://doi.org/10.1039/C3OB42096E

2013-2007

10. Vibrational self-consistent field calculations of spectroscopy of biological molecules
T. K. Roy and R. B. Gerber.
Phys. Chem. Chem. Phys. 15, 468 (2013). ISSN: 1463-9076,
https://doi.org/10.1039/C3CP50739D

9. A comparative study of independent particle model based approaches for thermal averages
S. Banik, **T. K. Roy** and M. D. Prasad,
J. Chem. Sci. 125, 1267 (2013). ISSN: 0974-3626,
https://doi.org/10.1007/s12039-013-0484-9

8. MOF-FF – A flexible first principles derived Force Field for Metal-Organic Frameworks
S. Bureekaew, S. Amirjalayer, M. Tafipolsky, C. Spickermann, **T. K. Roy**and R. Schmid
Physica Status Solidi (b) 250, 1128 (2013). ISSN: 1521- 3951,
https://doi.org/10.1002/pssb.201248460

7. Development of a new variational principle for thermal density matrices
T. K. Royand M. D. Prasad.
J. Chem. Phys. 134, 214110 (2011). ISSN: 1089-7690,
https://doi.org/10.1063/1.3592777

6. Functionalization of the terminal carbon atoms of the hydroxyl terminated polybutadieneby polyazido nitrogen rich molecules
R. M. Shankar, **T. K. Roy** and T. Jana
Bull. Mater. Sci., 34, 745 (2011). ISSN: 0250-4707,
https://doi.org/10.1007/S12034-011-0190-5

5. Terminal Functionalized Hydroxyl-Terminated: An energytic Binder for propellant
R. M. Shankar, **T. K. Roy** and T. Jana.
J. Appl. Poly. Sci. 114, 732 (2009). ISSN: 1097-4628,
https://doi.org/10.1002/APP.30665

4. On some strategies to design new high energy density molecules
T. Mondal, B. Saritha, S. Ghanta, **T. K. Roy**, S. Mahapatra and M. D. Prasad
Theochem, 897, 42 (2009). ISSN: 0166-1280,

https://doi.org/10.1016/j.theochem.2008.11.013

3. Effective harmonic oscillator description of anharmonic molecular vibrations
T. K. Roy and M. D. Prasad
J. Chem. Sci. 121, 805 (2009). ISSN: 0974-3626,
https://doi.org/10.1007/s12039-009-0095-7

2. A thermal self-consistent field theory for the calculation of molecular vibrational partition functions
T. K. Roy and M. D. Prasad.
J. Chem. Phys. 131, 114102 (2009). ISSN: 0021-9606,
https://doi.org/10.1063/1.3213568

1. Conformational preferences of mono-substituted cyclohydronitrogens: A theoretical Study
T. K. Roy, S. Ghanta, T. Mondal, B. Saritha, S. Mahapatra and M. D. Prasad.
Theochem, 822, 145 (2007). ISSN: 0166-1280,
https://doi.org/10.1016/j.theochem.2007.08.003

Book Chapter:

Development of Computational Tools forDiverse Applications of Metal Organic Frameworks: Challenges and Outlooks,
B. Danil, P. Kumar, A. Gondhi, **T. K. Roy** and K-H Kim
Chapter in a edited book. Central West Publishing,Australia, (2019) ISBN: 978-1-925823-57-8

Project Experiences

- Development of VSCF theory for large bio-molecules.
- Development of polarizable force-fields and its applications for breakable bonds as advancement of DL_POLY Classic code to molecular dynamic simulations.
- Developer of GAMESS quantum chemistry program package.
- Development of EHO approximation for molecular anharmonic vibrations.
- Development of a new method to molecular vibrational partition function and other thermodynamic state functions using thermal VSCF and EHO theory.
- Development of a new variational principle for thermal density matrices.
- Investigation of reaction mechanisms for biologically important reactions.

Collaborations :

- Prof. R. Benny Gerber, Fritz Haber Center for Molecular Dynamics Institute of Chemistry, The Hebrew University of Jerusalem, Israel.
- Prof. Oleg Boyarkin, Ecole Polytechnique Fédérale de Lausanne, Switzerland. (investigation of vibrational spectra of peptides)
- Department of Chemistry, Central University of Rajasthan.
- Department of Chemistry, Sastra Deamed University.

Teaching :

PhD Level: Advanced Quantum Mechanics, Computational Chemistry
M.Sc. Level: Quantum Chemistry, Group Theory and spectroscopy, Statistical Mechanics

B.Sc. Level: Quantum Chemistry, Chemical Kinetics, Solid State Chemistry, Mathematics for Chemist, Gas Laws, Thermodynamics, Electrochemistry, Spectroscopy

Computational Skills :

- FORTRAN, PYTHON scripting, SHELL scripting
- UNIX/Linux, Windows, Linux Cluster, Cray-XT super computer and IBM high performance computers.

Computational codes used :

- Gaussian, GAMESS, ORCA, MOPAC etc
- Material Studio, Discovery Studio, DL_POLY, TINKER etc

Software Development :

- Developer of GAMESS and other in-house software.

Selected Conferences, Oral and Poster Presentations :

Oral Presentation:

- Invited Talk: Theoretical Chemistry Symposium 2023, IIT Madras, 67-10 December
- Resource Person, Two-Week Online Faculty Development Programmein Chemistry and Allied Sciences – FDPCAS-2023,CU Jammu
- Invited Talk: Theoretical Chemistry Symposium 2019, BITS Pilani, 67-10 December
- Invited Talk: ERTSC, 2020, Govt. Post-Grad College, University of Jammu
- Invited Talk: ICIIHS, 2022, KLH University, Hyderabad
- Invited Talk: 2021, Amrita Viswa Vidiyaitham
- Oral Presentation: VI Rajasthan Science Congress, October 13-15, 2018 at Central University of Rajasthan.
- Invited Speaker: International Conference on Frontiers at the Chemistry-Applied Sciences Interface", Organized by University of Rajasthan, July-23-24, 2017, Title: Going solvated: Intrinsic Structures of a Micro-solvated Decapeptide Determined by Theory and Cold-ion Spectroscopy
- Invited Speaker: Theoretical Chemistry Symposium, TCS-2016, International Conference, 14th to 17th December, 2017, University of Hyderabad, IICT & IIIT, Hyderabad, Title: Conformationally Resolved Structures of Large Biological Molecules Validated by First Principles Based Anharmonic Calculations
- International Conference on Frontiers at the Chemistry-Applied Sciences Interface, April-25-26, 2016, University of Rajasthan, Title: Conformational Structures of a Decapeptide Validated by First-Principles Calculations and Cold Ion Spectroscopy
- J & K Science Congress, March 2-4, 2017 at University of Jammu, Title: Conformationally resolved 3d-structures and spectroscopy of large bio-molecules using quantum mechanical anharmonic calculations
- Advances in Chemical Sciences and Thermodynamics, December 2-3, 2016, University of Jammu, Title: Variational approach of thermodynamic quantities.
- '5th Singapore India Collaborative & Cooperative Chemistry Symposium', an international symposium organized by School of Chemistry, University of Hyderabad in 2009, titled - 'Variational approaches to thermodynamic quantities'.
- 7th Annual In-house Symposium organized by School of Chemistry, ChemFest 2010, titled – 'Effective Harmonic Oscillator Description of Anharmonic Vibrations'.

Poster Presentation:

- Poster presentation: "First-Principles Anharmonic Quantum Calculations for the Determination of Three-Dimensional Structures of Biological Systems" in Emerging Trends in Applied Chemical Sciences, March, 2016, Organized by Department of Chemistry, Central University of Rajasthan, India
- Poster presentation: 'First principle derived force for flexible reactive molecules', organized by Ruhr University, Bochum, Germany, 2012 at SFB 558 closing symposium.
- Poster presentation: 'Development of Polarizable Force Fields with Valence Charge Equalization method, in 14th International Conference on the theoretical aspects on Catalisys, Vlissingen, The Netherlands (2012).
- Poster presentation: 'A thermal self-consistent field theory for the calculation of molecular vibrational partition function': Recent Advances in Many Electron Theory, 2010; organized by Indian Association of the Cultivation of Science and Raman Centre for Atomic Molecular & Optical Science, Kolkata, India.
- Poster presentation: 'Calculation of thermodynamic quantities of molecules using effective harmonic oscillator and vibrational self-consistent field method': Theoretical Chemistry Symposium 2009, organized by Indian Institute of Science, Bangalore, India.
- Poster presentation: 4th, 5th, 6th and 7th Annual In-house Symposium of School of Chemistry, ChemFest 2007, 2008, 2009, 2010, organized by School of Chemistry, University of Hyderabad, Hyderabad, India, 2007, 2008, 2009 & 2010.
- Poster presentation: 'School of numerical quantum many body methods in Physics and Chemistry', organized by JNCASR, Bangalore, 2007.
- HPC Workshop for FIST Institutes conducted during February 19-22, 2007 with CDAC at Center of Modeling Simulations and Design (CMSD), University of Hyderabad.
- CMSD conducted lecture series on 'Simulations in Biology and Soft Matter' during 26th November-11th December 2007 at University of Hyderabad.
- CMSD Conducted HPC workshop on Tutorial 'Tools for Scientific Computing' during October 21-25, 2008 and NVIDIA TESLA Supercomputing Workshop on 30th July 2009.

Awards and Fellowships

- CSIR Junior Research Fellowship (JRF) – by qualifying the All India National Eligibility Test (NET) conducted by CSIR-UGC, INDIA, in 2005.
- Post-doctoral fellowship by SFB 558, Ruhr University, Germany.
- Received prestigious PBC fellowship for post doctoral research by Government of Israel.

Member:

1. CRSI, Co-convener JK Chapter, 2023
2. Life Member, CRSI, India