Curriculum Vitae of Saikat Roy

Name and Designation:	Saikat Roy Senior Research Fellow-IIT Kharagpur(2017-2023)
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Institution:	Indian Institute of Technology Kharagpur (IIT KGP)
Date of Birth:	09.12.1994
Gender (M/F/T):	M
Category (Gen/SC/ST/OBC):	Gen
Language (Speaking and Writing):	English, Bengali, and Hindi
Permanent Address:	Lapuria, Garhbeta, Paschim Medinipur, West Bengal, India-721127

Academic Qualification

Degree	Year	Subject	Unviersity/Institution	Marks (%)
10+2	2012	Science (major)	WBBCHSE	90.4
B.Sc (Honors)	2015	Chemistry (major) with Physics, Mathematics (minor), and English, Bengali (general)	Ramakrishna Mission Vidyamandira (Autonomous college under the University of Calcutta)	75.5
Masters (M.Sc.)	2017	Chemistry	IIT Kharagpur	86.6
Ph.D.	2017-2023	Computational Chemistry	IIT Kharagpur	-

Ph.D. Thesis	Incorporating Conformational Complexities in the Study of Reaction Mechanisms
Supervisor's Name	Dr. Anoop Ayyappan (Associate Professor, Department of Chemistry, IIT Kharagpur)
Institute	Indian Institute of Technology Kharagpur
Year of Award	Ph.D. defense held on June 2023

Research Interests:

Computational Chemistry, Complex Transition metal Catalysis and Organocatalysis Reactions, Automation in Reaction Mechanism, Electronic Structure and Chemical Bonding Analysis, Scientific Software Development, Machine Learning in Reaction Mechanism.

Software and Skills: Orca, Gaussian, Turbomole, PSI4, XTB, MOPAC, Chemshell (tcl and python), Multiwfn, Git, LaTeX,

Programming Languages: Python (primary), C++ (not expert), Bash

Open Source Projects: I have developed couple of opensource projects during my Ph.D. work

SSA:	Our implementation of Gillespie's Stochastic Simulation Algorithm Github Link: https://github.com/anooplab/ssa
rksn_automate:	Automation Script for Conformer Search and TS finding. Github Link: https://github.com/Saikat248/rksn_automate
anoopab-docs:	Beginners documentation/wiki for setting up various software in HPC Facility. Documentation is given according to PARAMSHAKTI Supercomputing Facility at IIT Kgp using (SLURM Queuing system) Website: https://anooplab-docs.readthedocs.io/en/latest/

Workshops and Conferences Attended up to Date:

- Workshop on "Machine Learning for Science (ML4SCIENCE)"(2018), IIIT Hyderabad, India.
- "Theoretical Chemistry Symposium (TCS)"(2021), Online Mode, IISER Kolkata, India, poster presentation.
- "National Conference on Molecular Modelling and Simulations (NCMMS)"(2022), Online Mode, VIT Bhopal, India, poster presentation.
- "Designing Catalysts on Computers (DCC)"(2022), IACS Kolkata, India, poster presentation.

Teaching Assistantship and Other Research Activities:

- Physical chemistry laboratory for first-year undergraduate students (2017, 2018).
- Introduction to Computational Chemistry course for M.Sc. students (2018).
- Physical chemistry laboratory for M.Sc. Students (2019).
- Introduction to Quantum Chemistry and Spectroscopy course for M.Sc. Students (2020).
- Supervised 2 M.Sc. project students and 3 junior research fellows in AnoopLab.
- Maintained AnoopLab cluster computing system at IIT Kgp (system administration).

Publications: (includes published, under preparation, and submitted)

Included in the thesis

1. *Insights into the Active Catalyst Formation from Di-nuclear Palladium Acetate in Pd Catalyzed Coupling Reactions: A DFT study;* **S Roy**, A Anoop, *The Journal of Physical Chemistry A*, **2022**, *126(46),* 8562-8576,DOI: https://doi.org/10.1021/acs.jpca.2c03762

2. *Rh(III)CatalyzedRegioselectiveSynthesisof[1,3]Oxazino[3,4-a]Indol-1-onederiva- tives: Tuning the reactivity towards Oxygen instead of Nitrogen, through Meyer-Schuster Rearrangement;* P Kumar, **S. Roy**, R Chandra, B Sridhar, A. Anoop, GV Karunakar, *Manuscript under preparation*
3. *Stereochemistry of the Benzylidene γ-Butyrolactone Dictates the Reductive Heck Cyclization Mode in the Asymmetric Synthesis of Aryltetralin Lignans: A Detailed Experimental and Theoretical Study*; B Sen, **S Roy**, S Garai, S Roy, A Anoop, S Hajra, **2022**, *87 (6),* 3910-3921, DOI: https://doi.org/10.1021/acs.joc.1c02174
4. *Exploring the Complexity of Proline-Based Organocatalyzed Asymmetric Michael Addition of β-nitrostyrene and Aldehyde with Automated Strategies;* **S Roy**, R Ramapanicker, A Anoop, *Manuscript Submitted*
5. *Significance of Conformational Analysis in the Study of Asymmetric Michael addition reactions of aldehydes to β-nitrostyrenes catalyzed by (S)-pyrrolidine-based organocatalysts;* **S Roy**, R Ramapanicker, A Anoop, *Manuscript Under Preparation*

Other publications

6. *Iridium (III)-Catalyzed Intermolecular Mild N-Arylation of Aliphatic Amides Using Quinoid Carbene: A Migratory Insertion-Based Approach;* S Bera, **S Roy**, SC Pal, A Anoop, R Samanta, *ACS Catalysis,* **2021,** 11*(17)*, 10847-10854, DOI: https://doi.org/10.1021/acscatal.1c02653
7. *$BAl_4Mg^{-/0/+}$: Global Minima with a Planar Tetracoordinate or Hypercoordinate Boron Atom;* M Khatun, **S Roy**, S Giri, SSR CH, A Anoop, VS Thimmakondu, *Atoms*, **2021,** *9 (4),* 89, DOI: https://doi.org/10.3390/atoms9040089
8. *Organomagnesium Crown Ethers and Their Binding Affinities with Li^+, Na^+, K^+, Be^{2+}, Mg^{2+}, and Ca^{2+} Ions – A Theoretical Study*; **S Roy**, K Thirumoorthy, UK Padidela, P Vairaprakash, A Anoop, , VS Thimmakondu, *ChemistrySelect*, **2021**, *6 (33)*, 8782-8790, DOI: https://doi.org/10.1002/slct.202102317
9. *Effect of ancillary ligand on DNA and protein interaction of the two Zn (II) and Co (III) complexes: experimental and theoretical study;* M Das, P Brandao, S S Mati, **S Roy**, A Anoop, A James, S De, U Das, S Laha, J Mondal, B Samanta, T Maity, *Journal of Biomolecular Structure and Dynamics*,**2021**, 1-16, DOI: https://doi.org/10.1080/07391102.2021.2001377
10. *Why an integrated approach between search algorithms and chemical intuition is necessary?* VS Thimmakondu, A Sinjari, D Inostroza, P Vairaprakash, K Thirumoorthy, **S Roy**, A. Anoop, W Tiznado, *Physical Chemistry Chemical Physics*, **2022**, *24 (19),* 11680-11686, DOI: https://doi.org/10.1039/D2CP00315E
11. *Performance of Density Functionals and Semiempirical 3c Methods for Small Gold–Thiolate Clusters;* M Khatun, S Paul, **S Roy**, S Dey, A Anoop, *The Journal of Physical Chemistry A,* **2023***, 127(10),* 2242-2257,DOI: https://doi.org/10.1021/acs.jpca.2c07561
12. *Wavelength Orthogonal and Rate Controlled Photorelease of Alcohol and Carboxylic Acids: Application for Dosage Controlled Delivery of Two Anticancer Drugs;* S Ray, **S Roy**, A Anoop, N. D. P. Singh, *Manuscript under preparation*

References:

- Prof. Anoop Ayyappan, Department of Chemistry, Indian Institute of Technology Kharagpur, Email: anoop@chem.iitkgp.ac.in
- Prof. Sabyashachi Mishra, Department of Chemistry, Indian Institute of Technology Kharagpur, Email: mishra@chem.iitkgp.ac.in
- Prof. Parag A. Deshpande, Department of Chemistry, Indian Institute of Technology Kharagpur, Email: parag@che.iitkgp.ac.in