

## 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	University/Institution	Marks (%)
10+2	2012	Science (major)	WBBCHSE	90.4
B.Sc (Honors)	2015	Chemistry (major) with Physics, Mathematics (minor), 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 May 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 a couple of open source 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](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 two M.Sc. project students and three junior research fellows in AnoopLab.
- Maintained AnoopLab cluster computing system at IIT Kgp (system administration).
- Reviewed one article in Chemistry – An Asian Journal.

**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)Catalyzed Regioselective Synthesis of [1,3]Oxazino[3,4-a]Indol-1-one derivatives: 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  $\gamma$ -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  $\beta$ -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  $\beta$ -nitrostyrene 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<sub>4</sub>Mg<sup>-0/+</sup>: Global Minima with a Planar Tetracoordinate or Hypercoordinate Boron Atom*; M Khatun, **S Roy**, S Giri, SSR CH, A Anoop, VS Thimmakondur, *Atoms*, **2021**, 9 (4), 89, DOI: <https://doi.org/10.3390/atoms9040089>
8. *Organomagnesium Crown Ethers and Their Binding Affinities with Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Be<sup>2+</sup>, Mg<sup>2+</sup>, and Ca<sup>2+</sup> Ions – A Theoretical Study*; **S Roy**, K Thirumoorthy, UK Padidela, P Vairaprakash, A Anoop, , VS Thimmakondur, *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 Thimmakondur, 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*

### Preprints

- *Insights into the Active Catalyst Formation from Di-nuclear Palladium Acetate in Pd Catalyzed Coupling Reactions: A DFT study*; **S Roy**, A Anoop, <https://chemrxiv.org/engage/chemrxiv/article-details/61f321ebe4d9b8f15bfa4fbc>

### **References:**

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