

DILAWAR SINGH SISODIYA

Contact Information

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Research Interests

- Light-matter interaction and its role in driving molecular dynamics.
- Excited-state processes and nonadiabatic Dynamics in photoactive systems.
- Theoretical foundations and comparative analysis of quantum chemistry methods.
- Computational exploration of Reaction Mechanisms.
- Development and application of electronic structure methods.

Education

- **PhD** in Theoretical/Computational Chemistry, BITS Pilani, K K Birla Goa Campus, 2020–2025
Advisor: Prof. Anjan Chattopadhyay
Thesis: A Computational Investigation on the Mechanisms of Template Synthesis and Trans-Cis Isomerization Reaction of Some Selected Crown Ethers[Submitted]
- **MSc** in Inorganic Chemistry, Maharaja Sayajirao University of Baroda, 2017–2019
- **BSc** in Chemistry, Maharaja Sayajirao University of Baroda, 2014–2017

PhD Research Summary

My doctoral research focuses on uncovering the mechanistic details of the template-assisted synthesis of selected crown ethers and the photochemical and thermal isomerization pathways of photoresponsive azo crown ethers. Using advanced electronic structure methods—DFT, TDDFT, and their spin-flip extensions (SF-TDDFT and MRSF-TDDFT)—I investigated both ground and excited-state potential energy surfaces (PES), locating critical features such as conical intersections to map plausible reaction pathways.

To support these studies, I developed custom Python and Bash tools for structure interpolation, automation, and pre-/post-processing of quantum chemical data. I also performed Molecular Dynamics simulations using xTB and MLatom to capture the behavior of reactive intermediates and isomerization events.

In parallel, I contributed to collaborative projects involving fluorescent molecular systems, where I explored photophysical phenomena such as Excited-State Proton Transfer (ESPT), Intramolecular Charge Transfer (ICT and TICT), Excited-State Intramolecular Proton Transfer (ESIPT), Aggregation-Induced Emission (AIE), Intersystem Crossing (ISC), and Spin-Orbit Coupling (SOC).

CURRICULUM VITAE

Technical Skills

- **Software:** Gaussian 16, GAMESS-US, ORCA, OpenMolcas, xTB, Mlatom, Newton-X
- **Programming Languages:** Python, Bash

Professional Experience

- **Senior Chemist**, Rubamin Pvt. Ltd. (3 months)
Project: Extraction of rare-earth elements from spent petroleum catalysts
- **MSc Dissertation** under Prof. R. N. Jadeja
Topic: DFT-based exploration of molecular properties of small molecules using Gaussian 09

Teaching Experience

- **Teaching Assistant** (2020–2024), BITS Pilani K K Birla Goa Campus
Responsibilities: Conducted undergraduate chemistry lab practical
Awarded 'Best Teaching Assistant'

Publications

1. **Sisodiya, D. S.**; Ali, S. M.; Chattopadhyay, A. Exploring the Reaction Pathway Involved in the Dibenzo-18-Crown-6 Synthesis from Catechol and Bis(2-Chloroethyl) Ether in Presence of Base. *J. Phys. Org. Chem.* 2022, *35* (3), e4309. <https://doi.org/https://doi.org/10.1002/poc.4309>.
2. **Sisodiya, D. S.**; Ali, S. M.; Chattopadhyay, A. A DFT Study on the Reaction Pathway Involved in the Metal-Ion-Templated Synthesis of Benzo-21-Crown-7(B21C7) from Catechol and Hexaethylene Glycol Ditosylate in the Presence of Base. *J. Phys. Org. Chem.* 2023, *36* (3), e4471. <https://doi.org/https://doi.org/10.1002/poc.4471>.
3. **Sisodiya, D. S.**; Ali, S. M.; Chattopadhyay, A. Unexplored Isomerization Pathways of Azobis(Benzo-15-Crown-5): Computational Studies on a Butterfly Crown Ether. *J. Phys. Chem. A* 2023, *127* (34), 7080–7093. <https://doi.org/10.1021/acs.jpca.3c02363>.
4. **Sisodiya, D. S.**; Chattopadhyay, A. The Photochemical Trans → Cis and Thermal Cis → Trans Isomerization Pathways of Azobenzo-13-Crown Ether: A Computational Study on a Strained Cyclic Azobenzene System. *J. Chem. Phys.* 2024, *161* (3), 34307. <https://doi.org/10.1063/5.0206946>.
5. **Dilawar Singh Sisodiya**, Anisha Mishra, Anjan Chattopadhyay. A Computational Study on the Thermal and Photo Isomerizations of Azobis(Benzo-15-Crown-5) Involved in the Potassium Ion Transport Across Organic Liquid Membrane (To be communicated 2025)
6. Chattopadhyay, A.; Menger, M. F. S. J.; **Sisodiya, D. S.**; Köppel, H. Theoretical Study of Spectroscopy and Photodynamics of Decatetraene as a Representative Dimethylated Polyene. *J. Phys. Chem. A* 2025, *129* (10), 2442–2453. <https://doi.org/10.1021/acs.jpca.4c08185>.
7. Shukla, A. K.; Choudhary, S.; **Sisodiya, D. S.**; Mahale, A.; Vipparthi, P.; Togiti, U. K.; Kulkarni, O. P.; Chattopadhyay, A.; Bhattacharya, A. Pyrrolo[1,2-a]Quinoxaline: A Combined Experimental and Computational Study on the Photophysical Properties of a New Photofunctional Building Block. *J. Phys. Chem. B* 2025. <https://doi.org/10.1021/acs.jpcc.5c01810>.
8. Shukla, A. K.; **Sisodiya, D. S.**; Savita; Chattopadhyay, A.; Bhattacharya, A. To Quench or Not: Extending a β-Carboline Fluorophore for TNT Detection in Aqueous Media via Simultaneous ESPT Destabilization and AIE. *J. Phys. Chem. B* 2023, *127* (46), 10025–10034. <https://doi.org/10.1021/acs.jpcc.3c05936>.
9. Bhosle, A. A.; Banerjee, M.; Hiremath, S. D.; **Sisodiya, D. S.**; Naik, V. G.; Barooah, N.; Bhasikuttan, A. C.; Chattopadhyay, A.; Chatterjee, A. A Combination of a Graphene Quantum Dots–Cationic Red Dye Donor Acceptor Pair and Cucurbit[7]Urill as a Supramolecular Sensor for Ultrasensitive Detection of Cancer Biomarkers Spermine and Spermidine. *J. Mater. Chem. B* 2022, *10* (40), 8258–8273. <https://doi.org/10.1039/D2TB01269C>.
10. Sen, S.; **Sisodiya, D. S.**; Nikam, R.; Chattopadhyay, A. Revealing the Unexplored Mechanism of Photochemical Oxaziridine Conversion Process of 2H-Imidazole 1-Oxides. *ChemistrySelect* 2022, *7* (41), e202202371. <https://doi.org/10.1002/slct.202202371>.
11. Sen, S.; **Sisodiya, D. S.**; Chattopadhyay, A. The Mechanism of Photoconversion of Cyclic Dinitrone to Oxaziridine and Dioxaziridine: A Computational Investigation of an Experimentally Reported Photochemical Reaction. *J. Phys. Org. Chem.* 2022, *35* (4), e4310. <https://doi.org/10.1002/poc.4310>.
12. Ashok Phadte, A.; Chattopadhyay, A.; Banerjee, S.; **Singh Sisodiya, D.**; Raghava, T. Synthesis of Green Emitting Multi-Substituted Dibenzodioxins and Related Heteroacenes and Computational Investigation

CURRICULUM VITAE

of Substituent Effects on Emission Spectra. *ChemistrySelect* 2020, 5 (33), 10177–10186. <https://doi.org/10.1002/slct.202001999>.

13. Sindhuja Sen, **Dilawar Singh Sisodiya**, Anjan Chattopadhyay, Photochemical Oxaziridine Conversion and Subsequent Lactam Formation Pathways of 3,5,5-trimethyl-1-pyrroline 1-oxide (3-Me-DMPO) *ISRAPS Bulletin* (2023)

Conferences and Workshops

1. Introduction to Gaussian: Theory and Practice, Hyderabad, India (Jan 2020)
2. NCMMS 2022, VIT Bhopal – Poster
3. NSRP-2023, BITS Pilani Goa Campus – Poster
4. TCS-2023, IIT Madras – Poster
5. Flash Talk: "The Molecular Dance of Butterfly Crown Molecules", BITS Pilani (Feb 2025)
6. CECAM55 Conference (Online), Sept 2024
7. Virtual Winter School on Computational Chemistry, University of Edinburgh (Jan 2025)
8. 57th Annual Convention of Chemists, 2020

Awards and Achievements

1. Cleared GATE (2019), GSET (2018)
2. Minaxi Lalit Award (3 times)
3. Best Teaching Assistant Award during PhD
4. Volunteered and helped organize academic events, including Open Science Day
5. Travel Grant award to attend **Theoretical Chemistry Symposium-2023 at IIT Madras**

Other Interests

Reading non-fiction books, especially philosophy and popular science.
Making music using Digital Audio Workstation.
Playing guitar with deep interest in Indian Classical music
