# KALYAN SINGH

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## OBJECTIVE

Versatile and research-oriented computational chemist with Ph.D. research focused on excited-state dynamics and photodissociation of small molecules, combining deep theoretical insight with practical simulation skills. Proficient in multireference quantum chemistry (CASSCF), nonadiabatic dynamics (SHARC), and electronic structure analysis (EDA-NOCV, QTAIM), with peer-reviewed publications in Chem. Asian J. and Dalton Trans.. Seeking opportunities in cutting-edge postdoctoral or R&D environments where fundamental understanding meets real-world application—ranging from photochemistry and catalysis to materials design. Adaptable, collaborative, and committed to contributing innovation across academic and industrial research landscapes.

## EDUCATION

**Ph.D| Banaras Hindu University**
2022 – Present
Board/University: Banaras Hindu University

**Ph.D| IISER Kolkata**
2019 – 2021
Board/University: Indian Institute of Science Education and Research Kolkata

**Post-Graduation | IIT Bombay**
2016 – 2018
Board/University: IIT Bombay CGPA: 7.4

**Graduation | Midnapore College**
2013 – 2016
Board/University: Vidyasagar University Percentage: 61.9 %

**12th Standard | Changual K. P. Vidyayatan**
2011 – 2013
Board/University: West Bengal Council of Higher Secondary Education Percentage: 73.0 %

## RESEARCH EXPERIENCE

For the past three years, I have been working on excited state dynamics, with a particular focus on the photodissociation dynamics of small molecules using trajectory surface-hopping techniques. My recent work on acetonitrile photodissociation was presented at TCS 2023. In parallel, I have contributed to computational studies on small molecule activation and bonding, with peer-reviewed publications in Chem. Asian J. and Dalton Trans., covering $CO_2$ reduction mechanisms and Y–Ge bonded yttrium germole dianion complexes. My current research continues to explore nonadiabatic pathways in molecular photodissociation dynamics.

## Publications

- *"Computational Exploration of Mechanistic Avenues in Metal-Free $CO_2$ Reduction to CO by Disilyne Bisphosphine Adduct and Phosphonium Silaylide"* Sayan Dutta, Kalyan Singh, Debasis Koley,* *Chem. Asian J.* 2021, DOI: 10.1002/asia.202100847

- *"Yttrium germole dianion complexes with Y-Ge bons"* Jingjing Liu,‡ Kalyan Singh, ‡ Sayan Dutta, Zhongtao Feng, Debasis Koley,* Gengwen Tan,* Xinping Wang, *Dalton Trans.*, 2021, *50,* 5552–5556. DOI: 10.1039/D1DT00798J

## Poster Presentation

- *"Photodissociation Dynamics of Acetonitrile at 121 nm: a Trajectory Surface-Hopping Study"*
  Kalyan Singh, Biswajit Maiti, * DOI: 10.13140/RG.2.2.24958.50247
  Date: 07 Dec 2023 - 10 Dec 2023
  Mode: Offline
  Conference Name: Theoretical Chemistry Symposium (TCS) 2023
  Organizing Institution: IIT Madras

- *"Computational Exploration of Mechanistic Avenues in Metal-Free $CO_2$ Activation by Disilyne Bisphosphine Adduct and Disilenes"*
  Kalyan Singh, Sayan Dutta, Debasis Koley, * DOI: 10.26226/morressier.614222345a6b32ccbe1480ef
  Date: 26 Sep 2021 - 29 Sep 2021
  Mode: Online
  Conference Name: 27$^{th}$ CRSI National Symposium in Chemistry
  Organizing Institution: IISER Kolkata

- *"Role of Disilene Substituents Toward $CO_2$ Activation: A Computational Study"*
  Kalyan Singh, Sayan Dutta, Debasis Koley, * DOI: 10.13140/RG.2.2.15846.55363/1
  Date: 01 May 2021 - 5 May 2021
  Mode: Online (twitter)
  Conference Name: RCS-IISER Desktop Seminar with PCCP
  Organizing Institution: IISER Thiruvananthapuram

## Master Project

Project title: Asymmetric Bis-allylation of Imines.
Objectives: To develop the asymmetric allylation of bis-imines by employing a chiral π-allylpalladium complex to furnish the bis-homoallylamines in good yields and enantioselectivity.
Project Duration: July 2017 - May 2018
Instructor: Prof. Rodney A. Fernandes
Institution: IIT Bombay

## TECHNICAL SKILLS

### Computational Chemistry Expertise:

- Proficient in excited-state dynamics, nonadiabatic simulations, electronic structure analysis, and bonding interpretation.
- Hands-on experience with advanced methods and techniques including: CASSCF, TDDFT, EDA-NOCV, NBO, QTAIM, and trajectory surface-hopping approaches.

### Software and tools:

- Quantum Chemistry Packages**: Gaussian, ADF, OpenMolcas, SHARC, AIMAll**
- **Visualization Tools**: GaussView, Chemcraft, Chemissian, CYLview, VMD, Molden, Mercury
- **Drawing and Reporting**: ChemDraw, ISIS Draw

### Programming & Technical Proficiency:

- Working knowledge of Python for data handling and automation in simulations.
- Familiar with HTML and basic web design.
- Comfortable working in Linux environments (Ubuntu, CentOS), Mac OS, and Windows OS.

## ACHIEVEMENT

- Qualified CSIR NET JRF Entrance Exam 2018
- Qualified GATE Entrance Exam 2018, 2019
- Qualified IIT JAM Entrance Exam 2016

## EXTRA CO-CURRICULAR ACTIVITIES

- **Languages Known**: English, Hindi, Bengali
- **Personal Interests**: Avid reader with a keen interest in science and technology trends. Enjoy playing badminton and engaging in intellectually stimulating discussions.
- **Personal Attributes**: Open-minded and receptive to new ideas, with a continuous drive for self-improvement. Known for maintaining a calm and composed demeanor under pressure, and for being adaptable, curious, and proactive in learning.

## PERSONAL INFORMATION

Date of birth: 2nd November 1995

Nationality: Indian

Religion: Hinduism

Sex: Male

Marital Status: Unmarried