

Omkar Chaudhari

First Year Graduate Student
Department of Chemistry
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EDUCATION

Degree	Institute	GPA	Year
PhD	University of Illinois Urbana-Champaign	4.0	2024 - Present
B.Tech Chemistry	Indian Institute of Technology, Guwahati, India	9.25/10	2020 - 2024

PUBLICATIONS

- 2025 **Interpretable Data-Driven Modeling on the Excited State Mechanisms of (Ni, Pt)-Centered Phosphorescent Materials - [Theoretical Chemistry Accounts \(Paper Link\)](#).**
Kaushik Soni, Omkar Chaudhari, and Kalishankar Bhattacharyya
- 2024 **A review of ensemble learning and data augmentation models for class imbalanced problems: combination, implementation and evaluation - [Expert Systems with Applications \(Paper Link\)](#).**
Azal Ahmad Khan, Omkar Chaudhari, and Rohitash Chandra

AWARDS AND HONORS

- Mr. Chinoree T. and Mrs. Kimiyo Enta Fellowship:** 2024
- Institute Silver Medal:** Awarded for graduating with the **highest grade** of the major.
- Institute Merit Scholarship:** Awarded for being the **highest grade scorer** and **Department Rank 1**.
- Techevince 8.0:** Team project won **Best Overall Project** in college's annual technical exhibition

COMPETITIONS

- Creative Shock:** Secured an **international rank of 14** in a global social business case study competition.
- Nexus Hackathon, Techniche IITG: Winner,** created an app to address logistic issues faced by hospitals.
- Respawn:** Runner up of the game development Jam hosted by 3 IITs for developing a tower-defence game.
- Spirit 2022:** Won **gold medal** as part of a water polo team representing our college at inter college event.
- Spardha 2023:** Won **3 Silvers, 2 Bronze medals** in aquatics in annual college inter hostel sport meet.

RESEARCH EXPERIENCE

- Graduate Researcher** Dec 2024 - Present
Supervisor: Dr. So Hirata Department of Chemistry, UIUC
 - Developing an ab-initio method for computing electron-phonon-electron interaction to formulate an ab-initio Frohlich Theory.
 - Implementing Coupled Cluster Theory to understand similarity transformation of Hamiltonian.
- Computational Materials Group** Sep 2023 - Jun 2024
Supervisor: Dr. Kalishankar Bhattacharyya Department of Chemistry, IIT Guwahati
 - Project 1:**
 - Developed a Python program for creating an automated computational workflow using **cheminformatics** and quantum chemistry to automate process of SMILES Strings to TD-DFT level calculations.
 - Project 2:**
 - Used Sure Independence Screening and Sparsifying Operator (SISSO) to generate useful features from a ground state DFT calculations dataset and predicted S1-T1 energy gap for (Ni, Pt)-Centered Phosphorescent Materials.
- Research Intern** Dec 2022 - Jun 2024
Supervisor: Dr. Usharani Dandamundi CSIR - Central Food Technological Research Institute(Remote)
 - Project 1:**
 - Probing Structure and Reaction Mechanisms of Microsomal Epoxide Hydrolases through **Multiscale Modeling** to Understand Lipid Signaling and Metabolism of EETs, EEQs, and EDPs to corresponding vicinal diols.
 - Used **Antechamber** to generate force field parameters, and performed **substrate docking** of xenobiotic fatty acids.
 - Project 2:**
 - Built **network representations** of Bifunctional **FAD Synthetase** using **NAPS**, performed **network analysis** and **shortest path analysis** of the apo and bound forms to investigate important residues for interdomain signalling.
 - Trajectory analysis using **MDAnalysis**, **Dynetan**, measuring key properties of protein network across snapshots such as **edge betweenness**, **node centrality**, and **length of shortest path** between active site residues of N-ter and C-ter Domains.
- Machine Learning Intern** Sept 2022 - Apr 2023
Supervisor: Dr. Rohitash Chandra University of New South Wales(Remote)
 - Evaluated **100** combinations of **data augmentation** and **ensemble techniques** on **30+ imbalanced** datasets.
 - Used **SMOTE**, **CTGANs**, **SMOTified-GAN**, and multiple bagging, boosting, voting, and stacking for classification.
 - Light Gradient Boosting Machine** along with various data augmentation techniques was found to outperform other combinations. Data augmentation techniques were found to be more influential over a dataset than classifiers.
- Undergraduate Thesis** Apr 2023 - Apr 2024
Supervisor: Dr. Chivukula V. Sastri Department of Chemistry, IIT Guwahati
 - Study of **C-S Bond formation** by **Cytochrome P450 enzymes** in Microbial sulphur-containing secondary metabolites.
 - Thorough investigation of substrate binding mode, role of key residues in substrate binding as well as catalytic activity of enzyme during the biotransformation using **molecular docking** and **molecular dynamics**.

TEACHING EXPERIENCE

- **CHEM 440 Principles of Physical Chemistry** Aug 24 - Present
Taught by: Dr. Christy Landes
 - Graded papers and held office hours during both Fall 2024 and Spring 2025. Created practice question sets each week.

CODING PROJECTS

- **Groww Simplex Route Optimization Problem** Jan 23 - Feb 23
Inter IIT Tech Meet 11.0 [Github](#)
 - Employed **Metaheuristic Techniques** to arrive to solutions for the **NP-Hard problem Capacitated Vehicle Routing Problem with Mixed Pickup and Delivery (CVRPMPD)**.
 - Created and Designed special **constraints and penalties** to lead the algorithm to certain solutions, considering parameters such as **Location Proximity, Delivery Dates, Capacity of Delivery Vehicles** etc.
 - Implemented the **sweep clustering algorithm** to break down the search space and solve sections individually, **reducing calculation time from 300 seconds to 60 seconds**, adding scalability to the solver to incorporate orders for large cities.
- **Job Shop Scheduling Modification** Oct 22 - Nov 22
Supervisor: Prof. Prakash Kotecha, Department of Chemical Engineering, IIT Guwahati [Github](#)
 - Modified the Job Scheduling Problem to remove start time from the decision variables and **reducing the search space**.
 - Assigned machine number to different orders using **metaheuristic techniques** such as **Genetic Algorithm, Particle Swarm Optimization, Ant Lion Colony Optimization** and a deterministic method optimized start times for orders.
 - **Multi-Objective Optimization** done using the **eps-constraint method** to optimize cost, makespan, and production time.
- **Oil Mixture Identification** Dec 22 - Dec 22
Supervisor: Dr. Usharani Dandamundi, CSIR-CFTRI, Mysore, India [Github](#)
 - Developed scripts to Identify Oil Compositions upto 5 different oils according to Fatty Acid standards from FSSAI.
 - The python scripts take inputs of Fatty Acid Values from a mass spectrometer, compares them to the permitted values of 20+ oils, and outputs an Excel Sheet containing possible compositions of the Oil Mixture.
- **NIR Spectra Classification** Aug 23 - Aug 23
Supervisor: Dr. Usharani Dandamundi, CSIR-CFTRI, Mysore, India [Github](#)
 - Classified different Millet Varieties from various Locations using **Principal Component Analysis**.
 - Combined **Principal Component Analysis** and **Linear Discriminant Analysis** to boost accuracy of separating the varieties.

COURSEWORK

- **Chemistry:** Molecular Electronic Structure Theory, Applied Quantum Chemistry, Advanced Quantum Chemistry, Computational Chemistry, Group Theory, Advanced Spectroscopy, Organometallic Chemistry, Nanomaterials, Statistical Mechanics, Chemical Data Science
- **Mathematics:** Linear Algebra, Computer Aided Optimization, Ordinary Differential Equations, Multivariate Calculus
- **Machine Learning and Deep Learning:** Neural Networks, Convolutional Neural Networks, Recurrent Neural Networks

TECHNICAL SKILLS

- **Softwares:** Gaussian09 (Scans, TDDFT, TS), ORCA (SOC)
- **Molecular Dynamics:** GROMACS, AMBER, Autodock Vina
- **Programming Languages:** Python, C++17, MATLAB, Fortran95
- **Libraries/Frameworks:** Numpy, Pandas, Tensorflow, Scipy, Seaborn, Matplotlib

LEADERSHIP ROLES

- **General Secretary**, Chemical Science and Technology Association, IIT Guwahati. July 2023 - May 2024
- **Branch Representative**, Department of Chemistry, IIT Guwahati. July 2021 - May 2024
 - Bridge between the Professors/Department Officials and the Students for Communication.
 - Organised internship talks by contacting alumni and professors.
- **Overall Projects Manager**, Coding Club IIT Guwahati. May 2022 - May 2023
 - Oversaw the successful completion of projects taken up by the Coding Club, from commercial to academic projects, with a funding of over 0.6 million INR.
 - Ran the club coding forum on discord with over 6000 members.
- **Aquatics and Water Polo Team Captain**, Mar 2023 - Apr 2023
 - Captain of the Aquatics and Water Polo team for Spardha Inter Hostel Sports Competition 2023.

EXTRACURRICULARS

- **National Service Scheme Volunteer**, July 2022 - Dec 2022
 - Attended workshops and talks on addressing the issues of corporal punishment and cyber bullying.
 - Picked up garbage from campus roads as part of a cleaning drive.
 - Took part in a national unity run organised by the National Service Scheme of India
 - Participated in a cleanliness drive in Maa Kamakhya Temple, Guwahati.
- **Events Executive of Cultural Festival, Alcheringa**, Dec 2020 - Mar 2022
 - Organised and Planned cultural events for the college cultural festival.
 - Contacted and signed international instrumentalists and theatre troupes for performances.
- **Workshops managing Team for Techniche**, Feb 2021 - Jan 2022
 - Organised workshops in domains for Cybersecurity, Machine Learning, Stock Markets.
 - Contacted and arranged for speakers during workshops.