



# Omkar Chaudhari

Roll Number: 200122042

B.Tech - Chemical Science and Technology

Indian Institute Of Technology, Guwahati

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## EDUCATION

Degree/Certificate	Institute/Board	CGPA/Percentage	Year
B.Tech.	Indian Institute of Technology, Guwahati, India	9.02 (Current) (Rank 1)	2020 - Present
Senior Secondary	ISC	90.8 %	2020
Secondary	Milton High School, Atlanta, USA	98.4 %	2018

## PUBLICATIONS

- 2023     **A review of ensemble learning and data augmentation models for class imbalanced problems: combination, implementation and evaluation** - [arxiv.org/abs/2304.02858](https://arxiv.org/abs/2304.02858).  
Azal Ahmad Khan, Omkar Chaudhari, and Rohitash Chandra

## ACHIEVEMENTS

- 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
- Creative Shock:** Secured an **international rank of 14** in the world's largest 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.

## EXPERIENCE

- Computational Materials Group** Ongoing  
IIT Guwahati  
Supervisor: Dr. Kalishankar Bhattacharyya, Department of Chemistry, IIT Guwahati
  - Developing a Python package for rapidly deploying automated computational workflow using **cheminformatics** and quantum chemistry. The package will automatically generate the XYZ coordinates from SMILES, and generate input files for **Gaussian**, **ORCA** for quantum mechanical calculations.
  - SMILES conversion done through **OpenBabel**, with conformer generation through **crest** and Semiempirical Tight Binding package **xtb**.
- Computational Materials Group** Ongoing  
IIT Guwahati  
Supervisor: Dr. Kalishankar Bhattacharyya, Department of Chemistry, IIT Guwahati
  - Creation of an extensive database utilizing **DFT**-computed data for organic chromophores.
  - TD-DFT** Calculations run along with **SOC** Calculations run in **ORCA** to compute rate of intersystem and reverse intersystem crossing.
  - We aim to employ a machine learning approach and automation protocol to forecast the properties of excited electronic states in organic molecules, drawing from this comprehensive database.
- CSIR - Central Food Technological Research Institute** Dec 2022 - Present  
Remote  
Supervisor: Dr. Usharani Dandamundi, Principal Scientist
  - 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.
- Computational review of State-of-the-Art techniques for Class Imbalance** Sept 2022 - Apr 2023  
Remote  
Machine Learning Intern - University of New South Wales
  - 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 project** Apr 2023 - Ongoing  
Supervisor: Prof. 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**.
  - Elucidating underlying C-S bond formation reaction mechanism through **P450 monooxygenase** in the biosynthesis of **sulphur-containing secondary metabolites** in microbes using **Quantum Mechanical (QM) cluster approach**.
- Job Shop Scheduling Modification** Oct 22 - Nov 22  
[GitHub](#)  
Supervisor: Prof. Prakash Kotecha, Department of Chemical Engineering, IIT Guwahati
  - 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.
- CSIR - National Chemical Laboratory** May 2022 - Jul 2022  
[GitHub](#)  
Supervisor: Dr. Amol A Kulkarni
  - Experimental Study of Impingement Dynamics of **Confined Impinging Jet Reactor** using flow visualization.
  - Used **OpenCV** for quantification of reaction progress of mixtures of solids by measuring red/green color ratio of images taken of a screw reactor.

## PROJECTS

- **Groww Simplex Route Optimization Problem** Jan 23 - Feb 23  
*Inter IIT Tech Meet 11.0*  
◦ 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.  
◦ **3D Bin Packing** was implemented for optimal packing of the deliveries in the rider's bag.  
[GitHub](#)
- **Campus Rush** Oct 21 - Mar 22  
*Coding Club IITG*  
<https://bit.ly/cmprush>  
◦ Created a **3D model** of IITG in **Blender**, along with **Multiplayer Functionality** and Online Leaderboard using **PHP APIs**.  
◦ Used **UV Unwrapping** to accurately texture models of various buildings of the college, modifying texture parameters like **roughness, diffusion, and normal maps** to give textures a realistic look while keeping performance requirements low.
- **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.

## TECHNICAL SKILLS

- **Softwares:** Gaussian09, ORCA, NAPS Network Analysis, Chimera, VMD, Molden, Chemcraft
- **Molecular Dynamics:** GROMACS, AMBER, Autodock Vina
- **Programming Languages:** C/C++, Python, MATLAB, Fortran
- **Libraries/Frameworks:** Numpy, Pandas, Tensorflow, Scipy, Seaborn, Matplotlib, MDAnalysis, Dynetan

## COURSEWORK

- **Chemistry:** Computational Chemistry, Quantum Chemistry, Group Theory, Advanced Spectroscopy, Organometallic Chemistry, Nanomaterials, Polymer Chemistry, Applied Organic Chemistry, Coordination Chemistry, Chemical Kinetics and Electrochemistry
- **Biology:** Introductory Biology, Fluorescence Techniques in Biotechnology
- **Mathematics:** Linear Algebra, Computer Aided Optimization, Ordinary Differential Equations, Multivariate Calculus
- **Machine Learning and Deep Learning:** Neural Networks, Convolutional Neural Networks, Recurrent Neural Networks

## LEADERSHIP ROLES

- **General Secretary**, Chemical Science and Technology Association, IIT Guwahati. July 2023 - Present
- **Branch Representative**, Department of Chemistry, IIT Guwahati. July 2021 - Present  
◦ Bridge between the Professors/Department Officials and the Students for Communication.  
◦ Managed 60 students, 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 projects to academic projects, with a funding of over 0.6 million INR.  
◦ Supervised 12 mentors across 10 projects and released projects in domains of Machine Learning, App Development, Web Development, and Cybersecurity, managing submission from over 400 teams.  
◦ Helped organise our first offline national hackathon, Ethos, with participants coming from all over India to the college, contacted companies and secured sponsorships worth 5 lakh.
- **Coding Forum owner**, Owner of **6000+** member discord server May 2022 - May 2023  
◦ Owner and Manager of a Coding Discord Server with 5000 members.  
◦ Released and conducted online courses and workshops.
- **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.  
◦ Managed a team of 14 people getting overall 2nd Place among all hostels in both Aquatics and Water Polo.

## EXTRACURRICULARS

- **Community Service**, 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 cell of my college.  
◦ Organised a cleanliness drive in a nearby temple.
- **Member of the Consulting and Analytics Club**, May 2021 - Apr 2022  
◦ Active member of the club, participated in many consulting national and international hackathons.  
◦ Part of active discussions and presentations on Neural Networks, applications of CNNs to image classification tasks.
- **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.  
◦ Ideated competitions and exhibitions for the college.
- **Workshops managing Team for Techniche**, Feb 2021 - Jan 2022  
◦ Organised workshops in domains for Cybersecurity, Machine Learning, Stock Markets for over 200 people.  
◦ Contacted and arranged for speakers during workshops.