

Dipesh Somvanshi

M.Sc. Chemistry (Computational Chemistry)

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📅 27th June 1997

☎ +91 8805143358

📍 Mumbai

SKILLS

Computational
Chemistry

Python

Neural Networks
from scratch

Gaussian

Experience with
Supercomputers

Organic Chemistry

Software De-
velopment

Basic Linux

Quantum
Mechanics

Basic Scripting

EDUCATION

M.Sc. Chemistry

🏛 Institute of Chemical Technology 📅 2018 – 2020

- Physical, Organic, Analytical and Inorganic Chemistry
- Course on Biochemistry in 3rd Semester
- Current GPA: 6.68 out of 10. Grade: BC

B.Sc. Chemistry

🏛 Ramnarain Ruia Autonomous College 📅 2016 – 2018

- Chemistry (Major), Physics (Minor), Mathematics
- GPA: 5.9 out of 7

MASTER'S THESIS

Theoretical Investigations and Predictions on the Catalytic cycle Mechanism of Pd/PTABS using DFT

Guide: Prof Anant Kapdi, Institute of Chemical Technology

Co-Guide: Prof Dilip Maity, Homi Bhabha National Institute (BARC)

Synthesis Collaborator: Prof Carola Schulzke, University of Greifswald, Germany

The project comprised of investigating the mechanism of recently developed catalyst by Kapdi Lab and predicting potential new structures for the next generation of catalyst. The catalyst was unique in nature due to a metal centre and 100+ atom count and a enzyme like behaviour. Various conformers were identified and initial reaction steps were analysed. The calculations were performed with Linux based Gaussian 16 on BARC supercomputer. Python was used for analysis. Experimental work was done by Siva Murty under Prof Carola Schulzke at Greifswald University, Germany.

EXPERIENCE

Institute of Chemical Technology

🏢 **Junior Researcher (Temporary)** 📅 Oct 2020 – Present 📍 Matunga Mumbai, Mumbai

Keywords: *Computational Chemistry*

Guide: Prof Anant Kapdi

- Investigation on backbonding and π -accepting nature of PTABS Ligand.

Tata Institute of Fundamental Research

🏢 **Junior Researcher (Temporary)** 📅 Jun 2020 – Dec 2020 📍 Colaba, Mumbai

Keywords: *Neural Networks, Computational Chemistry*

Guide: Prof Vamsee Voora

- Application of neural networks on conducting solid state materials.

Hertford College, Oxford University




🏢 **Junior Researcher (Collaboration)** 📅 Aug – Oct 2020 (3 Months) 📍 Ambarnath, Thane

Keywords: *Computational Chemistry, Python, Automation*

Guide: Prof Anant Kapdi **Collaborator:** Prof Fernanda Duarte

- Investigation of possibility of modelling Pd/PTABS system on recently developed autodE software by Prof Fernanda Duarte.

Homi Bhabha National Institute, BARC




 **Master Project Student**  Jun 2019 – Jun 2020 (1 year)  Anushakti Nagar, Mumbai
Keywords: *Computational Chemistry, Python, Supercomputer, Reaction Modelling*

Guide: Prof Anant Kapdi **Co-Guide:** Prof Dilip Maity

Synthesis Collaborator: Prof Carola Schulzke, University of Greifswald, Germany

- Worked on master thesis.
- Used Gaussian 16 with python and basic scripting, on a linux terminal of 300-core supercomputer.
- The system studied consisted of a organometallic catalyst with Palladium atom core and the catalyst size exceeding 100 atoms, unusual for a typical computational chemistry project.

Homi Bhabha National Institute, BARC

 **Intern**  May – Jun 2019 (2 months)  Anushakti Nagar, Mumbai
Keywords: *Computational Chemistry, Python*

Guide: Prof Dilip Maity

- Studied theory and application of Computational Chemistry.
- Used Gaussian 09 with python and basic scripting, on a linux terminal of 16-core cluster.




Seminar on “Use of Deep Neural Networks on predicting Molecular properties”

 **Master Student**  Dec 2019  ICT, Mumbai
Keywords: *Theory of Neural Networks*

Guide: Prof Jayshree Nagarkar

- Seminar included history and mathematics of Deep Neural Networks and current tools being employed for predicting molecular properties.
- The seminar was presented in front of an external referee.




Bachelor's Research Project

 **Bachelor Student**  May 2017 – March 2018 (10 months)  Ramnaraian Ruia AutoCollege, Mumbai
Keywords: *Microwave Synthesis, Organic Chemistry*

Guide: Prof Madhavi Badole

- Drastic reduction in reaction time with the use of formamide as a solvent and catalyst in microwave assisted knoevenagel synthesis of benzylidene malononitrile and it's effect on rate of reaction and percentage yield.

iWAB Solutions Pvt Ltd

 **iOS App Developer**  Jun – Aug 2016 (3 months)  Ambarnath, Thane
Keywords: *iOS App Development, Software Development, Objective C*

- Worked as part of a team in developing an app for a tourism company.
- Responsibility included partial development of front end and UI components of the software with a team member.

iWAB Solutions Pvt Ltd

 **Intern iOS App Developer**  Jan – May 2016 (6 Months)  Ambarnath, Thane
Keywords: *iOS App Development, Software Development, Objective C*

- Worked on various small projects.
- Responsibility included learning software development and contributing small snippets of code to various on-going projects.
- Worked with various team members in a collaborative environment.

PUBLICATIONS

A research paper in a reputed journal is currently in progress.
Draft of a paper on Cu system is being prepared.

OTHER ACTIVITIES

Head of Departmental Festival (*Rasayanam*) Event “Lab Tours”

Rasayanam 2019 and 2020

- The event consisted of PhD students of various labs demonstrating university lab instruments.
- Responsibility included getting permissions and coordinating with PhD students (and their guides).
- Responsibility also included working with teammates for proper crowd management and co-ordination.

Attended DAE Computational Chemistry Symposium

November 7-9 2019

- Attended poster presentations and lectures by various computational chemistry experts.

AWARDS

Homi Bhabha Young Scientist

2012

State-wide contest with a written and practical exam.

Gold Medalist (Karate)

2015

Winner of state level karate tournament with a spot on National Team.

LANGUAGES

Marathi

Mother tongue – Fluent

Hindi

National Language – Fluent

English

Working Language – Fluent

Japanese

Upper Intermediate Proficiency

German

Very Elementary Proficiency

HOBBIES

Learning Languages

Karate

Reading