House No. 646, 35th Lane IIT Kanpur, 208016 **J** +91 9935135006 ☑ r95g10@gmail.com **?** haozeke 🛩 rgoswami **⊕** Grimoire



# Rohit Goswami

"An unproblematic state is a state without creative thought. It's other name is Death." - David Deutsch

# Personal Data

Name Rohit Goswami

Date Of Birth 10.08.1995

Birthplace Brookhaven, New York, United States of America

# Work Experience

2019-PRESENT Department of Chemistry, Indian Institute Of Technology, Kanpur, Senior Project Associate.

I am affiliated to the Femtolab under the project "Femtosecond Laser Approaches to Quantum Information and Quantum Computation (SPO/MEITY/CHM/2018356)"

2018–2019 **Department of Chemical Engineering**, *Indian Institute Of Technology, Kanpur*, Project Associate.

I was associated with the Computational Nanoscience group. Over the course of two centrally funded projects, "Nucleation On Nanostructured Surfaces Computer Simulation Studies (SPO/DST/CHE/2017294)" and "Advanced Computation Research and Education (SPO/MHRD/CC/20130176)":

- o I worked on the implementation of an enhanced version of the CHILL (CHILL+) algorithm for tracking ice types.
- o Designed a linear discriminant analysis technique for near-surface ice structure determination which is undergoing rigorous testing
- Implemented a graph based network connectivity model for ice structures
- o Spearheaded the development of High Performance GPU accelerated molecular dynamics simulation anal-
- Worked on the determination of optimal GPU cluster configurations
- o Designed and administered academic outreach websites

### Education

2014–2018 B.Tech. Chemical Engineering, Harcourt Butler Technical University, Kanpur, India.

First Division (Project: Gas Sweetening Plant Design)

2011–2013 Intermediate (AISSCE), Delhi Public School Kalyanpur, Kanpur, India.

87.2% Central Board of Secondary Education (CBSE)

High School (AISSE), Delhi Public School Kalyanpur, Kanpur, India. 2009-2011

9.8 Cumulative Grade Point Average (CGPA) in Central Board of Secondary Education (CBSE)

# Voluntary Positions

2019-PRESENT IEEE P1940, IEEE Standards Committee, Working group member.

Am actively engaged in working with stake holders in industry and academia to create a collection of standard profiles that define integration of authentication services with ISO 8583 used for financial transactions.

2019-PRESENT R Novice Inflammation, The Carpentries, Maintainer.

As a maintainer for the Software Carpentries lesson on R, I work with the community to make sure that lessons stay up-to-date, accurate, functional and cohesive.

2019-PRESENT CarpentryCon 2020, The Carpentries, Program Committee co-chair & Website subcommittee

Working for an international conference with diverse leads from across the world, as part of the program committee I reached out to keynote speakers and managed the overall schedule. Wrote content with the website subcommittee and also contributed due to my web development expertise.

2019-PRESENT Univ.ai, Earth2Orbit Analytix Private Limited, Teaching Fellow and Developer.

Tested course-content and developed interactive labs to work with an online cohort of students. Am presently teaching labs and mentoring small batches. I also work with the front and backend teams to facilitate workflows including shopify stores and NodeJS authentication systems.

Animal Welfare Group, *Indian Institute of Technology Kanpur*, Member and Web-developer.

Have worked with student bodies to rescue and care for local animals. Also designed and maintain a site with ReactJS to enhance knowledge dissemination.

# Undergraduate Experience

## Internships

2017–2018 Dr. Debojit Chakrabarty, Keva Fragrances Ltd, Mumbai, R&D Industrial Intern.

Modeling complex multi-component perfumes in a predictive method via experimental and theoretical considerations. In collaboration with Prof. Rajdip Bandyopadhyaya of the ChemE Dept. at IIT Bombay.

Summer 2017 **Prof. Sibasish Ghosh**, *The Institute of Mathematical Sciences, Chennai*, Visiting Scholar.

Discussed computational techniques for the simulation and understanding of quantum tomography.

SUMMER 2017 Prof. Nisanth Nair, Indian Institute Of Technology Kanpur, SURGE Scholar.

An exploratory project to understand and deal with bottlenecks in computational chemistry, the major objectives were to investigate hybridization of existing code via OpenMP and MPI.

POSTER: Development of Computational Tools for Free Energy Calculations of Chemical Reactions

SUMMER 2016 **Dr. Rajarshi Chakrabarti**, Indian Institute Of Technology Bombay, Research Intern.

Retooled a server with ArchLinux and also simulated patchy colloids (Janus Particles).

PROJECT REPORT: Computational Survey of Coarse Grained Soft Matter Molecular Dynamics Simulations

# Volunteer Work

2017–2018 **ChemE Herald**, Harcourt Butler Technical University, Kanpur, Editor-in-Chief.

Inaugurated and managed an interdisciplinary technical newsletter.

2017–2018 HBTU-MUN 2018, Secretary General.

Designed a ReactJS based static website, with Trello backed user registration, also performed outreach preevents to raise awareness and participation, in addition to overseeing the working of the executive board.

2016–2017 **HBTU-MUN 2017**, Executive Board Chairperson.

Designed a Jekyll based static website and ensured adherence to standard MUN rules as Chairperson.

The Curiosity Magazine, Harcourt Butler Technical University, Kanpur, Editor-in-Chief. Managed a diverse team of student content writers and also later typeset a spin-off multi-lingual newsletter in  $X_{\exists}L^{A}T_{E}X$ .

#### **Technical Skills**

#### **Programming Languages**

EXPERIENCED CSS, JS, HTML, Sass, C, C++, R, FOR-TRAN, OpenMP, OpenMPI, Tcl FAMILIAR Ruby, Julia, Python, Shell (zsh, bash), Golang, ReactJS, Node, CUDA EXPERIENCED Android (Cyanogen, LineageOS, AOSP), Web-Design (static), Arch-

Linux

Simulation Projects

(Extensible EXPERIENCED ESPResSo Simulation

Package for Research on Soft matter), LAMMPS (Large-scale Atomic/Molecular Massively Parallel

Simulator)

**Tools** 

EXPERIENCED X<sub>3</sub>L<sup>A</sup>T<sub>E</sub>X, pandoc, Git (version con-

trol), tmux, ssh, Vim, Sublime Text Editor 3, gnuplot, gadfly, bspwm (tiling window manager), mosh, babun, MAT-LAB (matrix laboratory), Continuous Integration Services (Wercker, Travis

CI, Semaphore CI), docker

**Operating Systems** 

Preferred ArchLinux EXPERIENCED Windows (95, 2000, XP, 7, 8, 10), Ma-

> cOS (10.7, 10.11, 10.12), Android (1.5, 1.6, 2.2.\*, 2.3.\*, 4.0.\*, 4.4.\*, 5.0.\*, 6.0.\*, 7.\* ), Linux Distros (Ubuntu, Sabyon,

FAMILIAR Linux Kernel (Android)

namics)

FAMILIAR OpenFOAM, GROMACS (GROningen

FAMILIAR AWS (Amazon Web Services), moltem-

fice, LibreOffice)

MAchine for Chemical Simulations),

VMD (Visual Molecular Dynamics),

CPMD (Car-Parrinello Molecular Dy-

plate, jekyll, middleman, grunt, gulp,

Frameworks (Bourbon, Skeleton, neat)

Markup Languages (Textile, HAML,

Jade(pug)), Office-Suites (MS, OpenOf-

Puppy, Manjaro, Debian, Red Hat)

Opensource Contributions

CREATED PixN ROM & Kernel (AOSP based rom Mantained Xperia Z5 LineageOS (14.\*)

> for the Xperia Z<sub>5</sub>) HaoZeke's LineageOS

**Opensource Projects Created** 

ZENYODA Pandoc based, tup driven stand-alone DOCUYODA A document generation system based

> multi format (revealJS, beamer etc.) preon pandoc and latexmk driven by gulp sentation system with static site generawith yaml configuration and easy temtion.

plating.

STARDOCK Docker compose based containerized PYQTNUMSIM A Qt interface for verbose numerical

methods assignments. self-updating setup for media hosting, with traefik for reverse proxying.

sition and management.

GRIMOIRE Metalsmith and webpack based open source educational experiment with a strong focus on readabil-

ity, equations and references.

Includes music, ebook and video acqui-

Affiliations & Accolades

Memberships

2014-PRESENT **OSA (Optical Society of America)**, Student Member  $\rightarrow$  Early Career Member (2018).

2015-PRESENT AICHE (American Institute Of Chemical Engineers), Student Member → Young Professional

(2018).

2015-PRESENT APS (American Physical Society), Student Undergraduate Member → Early Career Member (2019).

2015-PRESENT IEEE (Institute of Electrical and Electronics Engineers), Student Member → Early Career Member

(2018).

2015-PRESENT **IOP** (Institute of Physics), Student Member (2018) → Member (2019).

2006-PRESENT World Taekwondo, Red Belt.

2009-PRESENT XDA Developers, Senior Member.

2019-PRESENT AAAI (Association for the Advancement of Artificial Intelligence), Professional Member.

2019-PRESENT ACM (Association for Computing Machinery), Professional Member.

Also part of the SIGHPC (Special Interest Group for High Performance Computing) & SIGHPC-Education

2019-PRESENT ASAPBio (Accelerating Science and Publication in biology), Ambassador.

2019-PRESENT IChemE (Institute of Chemical Engineers), Associate Member.

2019-PRESENT IEEE IAS (Industrial Applications Society), Member.

2019-PRESENT IEI (The Institution of Engineers [India]), Associate Member.

2019-PRESENT InRaSS (Indian Radio Science Society), Student Member.

2019-PRESENT OSI (Open Source Initiative), Individual Member.

2019-PRESENT OSI (Optical Society of India), Life Fellow.

2019-PRESENT SPIE (Society of Photo-Optical Instrumentation Engineers), Early Career Professional.

2019-PRESENT **The Carpentries**, Certified Instructor.

2019-PRESENT URSI (Union Radio-Scientifique Internationale), Corresponding Member.

#### **Awards**

DECEMBER Photonics-2016, Indian Institute Of Technology Kanpur, Springer Best Student Paper Award,

2016 Nonlinear-Optics Session.

2014–2015 IITG Zephyr Creative Writing, Indian Institute Of Technology Guwahati, First Prize.

2014–2015 Antaragni IITK-MUN GA-DISEC, Indian Institute Of Technology Kanpur, Best Speaker.

#### Reviews

## 2018-PRESENT Journal Of Open Source Software, Reviewer.

I review submissions pertaining to molecular dynamics, virtualization, HPC, web platforms, finite element methods, optimization and computer geometry written primarily in C++, Rust, FORTRAN, Julia, Javascript. I am also listed for Python and R submissions. Specifically:

- o DEPP Differential Evolution Parallel Program
- RHEOS A Julia package for Rheology Data Analysis
- o Computing diffusion coefficients in macromolecular simulations: the Diffusion Coefficient Tool for VMD
- o Simple-Web-Server: a fast and flexible HTTP/1.1 C++ client and server library
- HyperNaut: a navigator for the hyperbolic plane
- The Biddy BDD package
- Prest: Open-Source Software for Computational Revealed Preference Analysis

2019-PRESENT PeerJ - Life & Environment, Reviewer.

2019-PRESENT **PeerJ - Computer Science**, Reviewer.

2019-PRESENT PeerJ - Organic Chemistry, Reviewer.

2019-PRESENT PLOS ONE, Reviewer.

# Publications

#### **JOURNALS**

Rohit Goswami, Amrita Goswami, and Jayant Kumar Singh. "d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations." In: *Journal of Chemical Information and Modeling* (Mar. 2020). ISSN: 1549-9596. DOI: 10.1021/acs.jcim.0c00031. URL: https://doi.org/10.1021/acs.jcim.0c00031.

Rohit Goswami. "Don't Pull Punches in Peer Review." In: *Nature* 574 (Oct. 8, 2019), pp. 176–176. DOI: 10.1038/d41586-019-03024-2. URL: /articles/d41586-019-03024-2 (visited on 10/09/2019).

Prerna, Rohit Goswami, Atanu K. Metya, S. V. Shevkunov, and Jayant K. Singh. "Study of Ice Nucleation on Silver Iodide Surface with Defects." In: *Molecular Physics* (Aug. 25, 2019), pp. 1–13. ISSN: 0026-8976, 1362-3028. DOI: 10.1080/00268976.2019.1657599.

#### Conference Proceedings

R. Goswami and D. Goswami. "Quantum Distributed Computing with Shaped Laser Pulses." In: 13th International Conference on Fiber Optics and Photonics (2016). DOI: 10.1364/photonics.2016.w4c.3.

R. Goswami, A. Goswami, and D. Goswami. "Space Filling Curves: Heuristics For Semi Classical Lasing Computations." In: 2019 URSI Asia-Pacific Radio Science Conference (AP-RASC). Mar. 2019, pp. 1–4. DOI: 10.23919/URSIAP-RASC.2019.8738612.

#### **PREPRINTS**

Nairhita Samanta, Rohit Goswami, and Rajarshi Chakrabarti. *Diffusion of self-propelled Janus tracer in polymeric environment*. 2017. arXiv: 1704.06207.

Rohit Goswami, Amrita Goswami, and Jayant K. Singh. *d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations*. 2019. arXiv: 1909.09830.

## Conference Records

#### **Posters**

- MARCH 2020 **Ultrafast Insights for Predictive Fragrance Compounding**, *ACS Spring 2020 National Meeting*, R. Goswami, A. K. Rawat, D. Chakrabarty, and D. Goswami, Accepted.
- DECEMBER **Qubit Network Barriers to Deep Learning**, *IEEE WRAP-2019*, R. Goswami, A. Goswami, and D. 2019 Goswami.
- MARCH 2019 **Space Filling Curves: Heuristics For Semi Classical Lasing Computations**, URSI Asia-Pacific Radio Science Conference (AP-RASC 2019), R. Goswami, A. Goswami, and D. Goswami.
  - DECEMBER FDTD Numerical Computations for Ultrafast Non-linear Optics, *Photonics-2018*, R. Goswami, A. 2018 Goswami, and D. Goswami.

#### **Oral Presentations**

- DECEMBER Process Safety in terms of Latent Dirichlet Allocations, 72nd Annual Session of of the Indian Institute of Chemical Engineers, CHEMCON-2019, R. Goswami, Accepted.
- October 2019 Semi-Supervised Approaches to Ultrafast Optimal Control Theory, 43rd Symposium of the Optical Society of India, International Conference on Optics & Electro-Optics, R. Goswami, A. Goswami and D. Goswami.
  - DECEMBER Quantum Distributed Computing with Shaped Laser Pulses, 13th International Conference on 2016 Fiber Optics and Photonics, R. Goswami and D. Goswami.

# Workshops

- October 2019 **TriangleSCI 2019**, *Invited to the Triangle Scholarly Communication Institute*, A week long fully-funded incubator to discuss actionable goals towards Bringing Equity and Diversity to Peer Review. This was undertaken as part of the larger discussion on Equity in Scholarly Communications, **declined to attend**.
- MAY-JUNE 2019 **Artificial Intelligence**, *E & ICT Academy*, *IIT Kanpur*, A four week course on AI foundations culminating in a time-series prediction project.
  - JUNE 2019 **AI Foundations Certificate Course**, *univ.ai*, A summer school taught in-person by faculty from Harvard and UCLA, culminating in a computer vision and neural network based identification project.
  - JULY 2019 Rare Events Summer School, *Indian Institute of Science, Bangalore*, A short course consisting of lectures and hands-on sessions by experts in the field, organized by Prof. Baron Peters.

**Short Courses** 

September 23<sup>rd</sup> Surface Area and Porous Material Characterization, *Dept. of ChemE, IIT Kanpur*, An intensive day long course on the basics of experimental classification and DFT methods for pore distribution by Dr. Martin Thomas from Anton-Paar.

September 21st OpenACC GPU Bootcamp, Chemistry Department, IIT Kanpur, Day long programming session and discussion covering the acceleration of Institute in-house code facilitated by a Senior Nvidia Solution Architect (Mr. Bharatkumar) and Prof. Debabrata Goswami.

# Certifications

## **NPTEL Courses**

 $\label{eq:Jan-Apr-2019} \textbf{Graph Theory}, \textit{IISER Pune}, 55\%.$ 

License: NPTEL19MA13S21460067

Aug-Sep 2018 Computational Chemistry and Classical Molecular Dynamics, IIT Bombay, Elite, 77%.

License: NPTEL18CS13S21440127

Aug-Sep 2018 Introduction to Parallel Programming in OpenMP, IIT Madras, 40%.

License: NPTEL18CS55S11440122

Jan-Apr 2018 **Quantum Computing**, *IIT Kanpur*, Elite, 65%.

License: NPTEL18CY07S4480024