Aayush Gupta, PhD

2125 Biscayne Blvd #400E, Miami, FL, 33137
♦aayush.ict@gmail.com ♦+1 (773) 658 2050 ♦Homepage ♦LinkedIn ♦Scholar ♦GitHub

SUMMARY

Aayush is an innovative computational chemist with over 9 years of combined academic and industrial experience. His research focuses on the integration of AI with cutting-edge quantum and classical molecular modeling techniques. Aayush possesses a diverse skill set that includes computer programming, data science, and expertise in building Linux servers and GPUs. He has a strong background in developing computational workflows for electronic structure and protein-drug modeling, demonstrating entrepreneurial and independent research skills throughout his career. Aayush has a proven track record of publishing as a first author in peer-reviewed journals, showcasing his ability to generate new ideas, develop prototypes, and document his findings. With a deep passion for continuous learning and implementing innovative techniques, he is dedicated to pushing the boundaries of scientific advancements.

EDUCATION

University of Illinois at Chicago
- Doctor of Philosophy *(Computational Chemistry)* — *Aug'16 – Feb'22*
  - Advisor: Prof. Huan-Xiang Zhou
- Master of Science *(Chemistry)* — *Aug'16 – Dec'18*

Institute of Chemical Technology, Mumbai, India
- Bachelor of Technology *(Chemical Technology)* — *Aug'12 – May'16*

RESEARCH EXPERIENCE

AI Research Scientist | **Exscientia Inc** — *Mar'22 - Current*
- Collaborating with the AI-ML team to expedite drug discovery processes by developing hybrid AI/QM/MM methods.
  - Discovered neural network potential (NNP) outperforming state-of-the-art ANI; achieving accuracy of coupled-cluster theory and validated on dimer-interaction (DE Shaw Research) dataset.
  - Enhanced efficiency of torch models (GNN-NNP) by reimplementing them to optimize performance on multi-GPUs and wrapping in automated workflow.
- Involved in independent research projects, contributing to approximately 20% of job responsibilities.
- Engaged in ongoing communication with medicinal/organic chemists to identify potential clinical drug candidates and improve AI models through redesign.

Ph.D. Research | Title: "Machine Learning Methods for Advancing Computational Chemistry"
- Designed an efficient workflow for drug discovery by integrating a hybrid neural network (pseudo-quantum) and classical forcefields-based molecular dynamics simulations against COVID-19 main protease (M^{PRO}).
- Developed an ML-enabled pipeline for large-scale virtual drug screening using clustering and deep learning in combination with physics-based approaches against RPN11 - a drug target for breast cancer.
- Implemented an AI-based generative deep network to guide conformational sampling of intrinsically disordered proteins (IDPs). Proposed a protocol to accelerate (learn and generate) MD simulations.
- Other areas: QM modeling of electron transport in peptide helices subject to chirality-induced spin selectivity (CISS) effect and its application in protein-protein interaction.

Research Internship | **Schrödinger Inc, NYC** — *Summer'19*
- Evaluated performance of deep neural network potentials (ANI) to achieve DFT(QM) accuracy at force-field speed (100x) for small molecule crystal polymorph prediction. Reported 98% DFT-ANI correlation in prediction.
- Analyzed potential energy surfaces of 100 different crystal structures (over 500 polymorphs) using DFT/ANI-1 potentials and identified their experimental stable forms (from an exhaustive literature search).

Research Assistant | UIC | *Advisor Dr. Petr Král* — *Aug'16-Dec'17*
- Performed quantum chemistry calculations | QM techniques used: DFT, TDDFT, QMMM, AIMD, PES, Electron Transfer, Molecular Orbitals, NBO, ESP, NMR, Spectra, QST2, CASSCF.

Previous Research Internships | Undergraduate
- Moscow Institute of Physics and Technology, **Moscow, Russia** | *Advisor: Prof. Artem Oganov* — *Jun-Aug'15*
  - Predicted stable/metastable structures of Europium Nitride (Eu_2N) crystal (using USPEX)
- Indian Institute of Sciences (IISc), Bengaluru | *Advisor: Prof. S Yashonath* — *May-Jun'15*
  - Performed molecular dynamics simulations of Zeolite MOF with warfare agents (xylene, benzene etc)
- Bhabha Atomic and Research Centre, Mumbai | *Advisor: Prof. Swapan Ghosh* — *Dec-Jan'15*

- Carried out periodic DFT on novel porous carbon nitride (C_3N_4) to investigate water splitting reactions.

- National Institute of Interdisciplinary Science and Technology (CSIR) | *Advisor: Dr. CH Suresh* *May-Jul'14*
  - Modeled reaction isomerization path (cyclopropene to allene) using first principle methods (DFT).
- Institute of Chemical Technology | *Advisor: Prof. N. Sekar* *Jan-May'13*
  - Predicted color of dye molecules using theoretical calculations - particle in a box/ring methods.

Undergraduate Research | ICT, Mumbai
- Thesis titles: "Dyeing with Fluorescent Dyes" | "Computational insight into possible dehydrated and depolymerized mechanisms of cellulose" | *Advisor: Dr. U Sayyed* | Grade: A
- Unforeseen bending in 1D silicene layers | Yearlong work in Prof. VG Gaikar group | (paper)

Industrial Experience | **Crystal Chemicals, Mumbai** | In-Plant Trainee | *Summer'14*
- Work Description: Synthesis workflow of industrial auxiliaries and chemicals (wet-lab experiments)

COMPUTATIONAL SKILLS

- *Data Science:* Machine Learning methods: Clustering, SVM, Decision Tree, Neural Network, Autoencoders, Generative Adversarial Network (GAN), and other Deep Learning methods.
- *Computer Enthusiast:* **Playing admin role** in troubleshooting system-related issues in our research group • Designed LDAP-based client-server protocol (400 TB file server+10 clients) • Experience with Linux architecture (*Networking, Security and File server)* • GPU benchmarking of simulation packages.
- *Scientific Programming*: Python, bash, and tcl (graphical) scripts.
- *Python Tools & Modules:* Pandas, NumPy, Keras, Tensorflow, Sklearn, Seaborn, Matplotlib, SciPy, Atomic Simulation Environment (ASE), Docker and Pytorch.
- *Schrödinger Suite:* Potentially explored backend workflow of various packages during the summer internship.
- *Simulation Packages*: **MD:** NAMD, AMBER, DL-POLY, Gromacs, Desmond • **QM:** Siesta, Gaussian16, Orca, Terachem, GAMESS, VASP, USPEX, Quantum-Espresso • **Docking:** Autodock, Glide, Gold, DLscore, Pafnucy.
- *Visualization:* VMD, Pymol, Chimera, Molden, Gabedit, Gaussview, VESTA, Avogadro, Mercury.
- *Cheminformatics:* RDKit, OpenBabel, PaDel, Balloon, and Confab (for generating drug conformations)
- *Biochemistry skills*: Protein purification, X-ray crystallography, and CyroEM

PUBLICATIONS & PRESENTATIONS

1. Gupta, Aayush, Dey, Souvik, Hicks, Alan, Zhou, Huan-Xiang (2022). Artificial intelligence guided conformational mining of intrinsically disordered proteins. Nature Commununications Biol, 5, 610. **[**PDF**]** **[**News**]**
2. Gupta, Aayush and Zhou, Huan-Xiang. (2021). Machine Learning-Enabled Pipeline for Large-Scale Virtual Drug Screening. *Journal of Chemical Information and Modeling*, 61, 9, 4236-4244. **[**PDF**]** **[**News**]**
3. Gupta, Aayush and Zhou, Huan-Xiang. (2020). Profiling SARS-CoV-2 main protease (M^{PRO}) binding to repurposed drugs using molecular dynamics simulations in classical and neural network-trained force fields. *ACS Combinatorial Science*, 22(12), 826-832 **[**PDF**]**.
4. Gupta, Aayush (2020). Profiling molecular simulations of SARS-CoV-2 main protease (M^{PRO}) binding to repurposed drugs using neural network force fields. ChemRxiv
5. Gupta, Aayush and Arora, Jyotsna S. (2017). DFT evidence of unforeseen bending in linearly fused polycyclic rings of Hexasilabenzenoids. *Computational and Theoretical Chemistry*, 1099, 87-91. **[**PDF**]**

ORAL & POSTER PRESENTATIONS:

6. Gupta, Aayush, Oral Presentation, ACS Meeting, San Francisco, USA. (Apr'17).
7. Gupta, Aayush, Poster Presentation, "Modelling of CO_2 Reduction in Ionic Liquid Catalysed by Oxygen" Annual Midwest Theoretical Conference, East Lansing, MI, USA (Jun'17).

REVIEWER / TEACHING EXPERIENCE

Reviewer: **Journal of Computational Biology**, *Mary Ann Libert Inc Publishers (verified)*

Teaching Assistantship:
- Physical Chemistry for Biochemists I *(Fall'18)*; CHEM340; Thermodynamics
- Physical Chemistry I & II *(Fall'17 & Spring'18);* CHEM 342 & CHEM346: Quantum Chemistry, Statistical Thermodynamics, Spectroscopy, Computational Chemistry
- General Chemistry I & II *(First Year);* CHEM122, CHEM123, CHEM124 & CHEM125.

Duties: Primary instructor in wet labs | Lead discussion classes | Grader | Problem solving hours

ADVANCED COURSES

1. Program Design/Data Structure
2. Introduction to Data Analysis *(CHEM594)*

3. Advanced Biochemistry *(CHEM550)*
4. Advanced Inorganic Chemistry *(CHEM520)*
5. Quantum Mechanics *(CHEM542)*
6. Molecular Spectroscopy *(CHEM543)*
7. Overvw of Computation in Phys *(PHYS491)*
8. Biophysical Methods *(CHEM557)*
9. Python for Biochemists *(CHEM557)*
10. *Mol & Cellular Biophysics (PHYS594)*

AWARDS & EXTRACURRICULARS

- Two-time recipient of **Chancellor's Student Service and Leadership Award** at UIC *(Apr'20 & Apr'22)*
- Best **TA Award** for General Chemistry II Discussion & Lab (CHEM124/125) *(May'18)*
- Received ***"GSC Travel Award"*** and ***"Student Presenter Award"*** at UIC *(2017)*
- Organized "Chicago Biophysical Networking Event" at UIC on (*Sep'19)*
- Active mentor at Science Club by Northwestern University.
- Panellist at the event ***"Graduate School Reality Check"*** at ACS meeting at San Francisco.
- Shortlisted among the invitees to attend *"Indian Science Academies Workshop"* **BIT-Mesra**, Deoghar.
- Awarded 5top100 scholarship to work at **MIPT, Moscow, Russia**. *(% intake : 5)*
- Awarded **Indian Academies of Sciences** - Summer Research Fellowship. *(% intake : 2)*
- **Diploma in Computer Application** (DCA) from Public University, India with A+ grade.
- Presented topic **"Darwin Awards"** at IGNITE (20 slides in 5 mins) | Invited **speaker** at *Freshers event* at ICT
- Hobbies: Badminton, Marathon Runner | Poker champion @ Schrödinger Poker Night.