

# Aayush Gupta, PhD

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## 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.

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## 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

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## 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.
- 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<sup>PRO</sup>).
- 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<sub>2</sub>N) 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<sub>3</sub>N<sub>4</sub>) 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)

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## 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 CryoEM

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## PUBLICATIONS & PRESENTATIONS

1. [Gupta, Aayush](#), Dey, Souvik, Hicks, Alan, Zhou, Huan-Xiang (2022). Artificial intelligence guided conformational mining of intrinsically disordered proteins. [Nature Communucations 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<sup>PRO</sup>) 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<sup>PRO</sup>) 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<sub>2</sub> Reduction in Ionic Liquid Catalysed by Oxygen” Annual Midwest Theoretical Conference, East Lansing, MI, USA (Jun'17).

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## REVIEWER / TEACHING EXPERIENCE

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

### Teaching Assistantship:

- o [Physical Chemistry for Biochemists I](#) (Fall'18); CHEM340; Thermodynamics
  - o [Physical Chemistry I & II](#) (Fall'17 & Spring'18); CHEM 342 & CHEM346:  
Quantum Chemistry, Statistical Thermodynamics, Spectroscopy, Computational Chemistry
  - o [General Chemistry I & II](#) (First Year); CHEM122, CHEM123, CHEM124 & CHEM125.
- Duties: Primary instructor in wet labs | Lead discussion classes | Grader | Problem solving hours

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## ADVANCED COURSES

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| 1. Program Design/Data Structure           | 6. Molecular Spectroscopy (CHEM543)        |
| 2. Introduction to Data Analysis (CHEM594) | 7. Overvw of Computation in Phys (PHYS491) |
| 3. Advanced Biochemistry (CHEM550)         | 8. Biophysical Methods (CHEM557)           |
| 4. Advanced Inorganic Chemistry (CHEM520)  | 9. Python for Biochemists (CHEM557)        |
| 5. Quantum Mechanics (CHEM542)             | 10. Mol & Cellular Biophysics (PHYS594)    |

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## AWARDS & EXTRACURRICULARS

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- 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.