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 focus is at the nexus of AI, Physics and Chemistry, he seamlessly integrates AI into advanced quantum and classical molecular modeling. He is proficient in machine learning, programming, and data science, and is well-versed with AWS, Linux servers, and GPUs. Aayush has a strong background in developing ML-based computational workflows for solving molecular properties and protein-drug modeling. He has consistently displayed entrepreneurial and independent research skills throughout his career. He 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. Passionate about learning and innovation, Aayush is committed to pushing *"AI for Science"* forward.

VISA Status: H1b approved (valid till 2029)

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*

- Working with the AI-ML team to expedite drug discovery by developing hybrid AI/QM/MM methods. Leading PhysicsML team (within ML team).
  - Discovered graph-based neural network potential (EXS-NNP) outperforming state-of-the-art ANI on coupled-cluster theory dataset, recognized as a significant *breakthrough* at Exscientia.
  - Enhanced efficiency of NNPs by reimplementing them for multi-GPU training and predictions, automated training workflow, and integrated for conformer generations and MD simulations.
  - Research project (10% innovation): "Fusing Force-Field Features within GNNs": Crafted a novel message-passing GNN architecture bridging AI & Physics, predicting fast and accurate energies/binding-affinity.

- Bridging the gap between ML teams and chemists by actively engaging with medicinal chemists to refine AI models based on their feedback.
  - Projects involved: Diffusion Model Based Docking; to mitigate protein-ligand clashes.
    Active Learning for Compound Selection: to refine binding free energy predictions,
  - Implemented a docking workflow to generate 3D structural features, and integrating these features with 2D ADMET models, resulting enhanced overall performance.
  - Successfully reintroduced Deep Learning based AI-based linker generation between two fragments, resulting in the submission of two molecules for synthesis and *in-vitro* assays.

Ph.D. Research | Title: "Machine Learning Methods for Advancing Computational Chemistry"
- Implemented a generative AI deep network for conformational sampling of intrinsically disordered proteins (IDPs) introduced a protocol to accelerate MD simulations. (github)
- Developed an ML-driven pipeline for large-scale virtual drug screening, combining clustering, deep learning, and physics-based methods against the RPN11 breast cancer target (github)
- 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}).
- 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.
    - Acknowledged in *Inorg. Chem.* 2019, 58, 16, 10516–10526

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)

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**]**

COMPUTATIONAL SKILLS

AI/ML & Data Science Skills

- AI & Machine Learning: Equivariant GraphNNs, Deep Learning, Generative Autoencoders & Adversarial Network (GAN), Diffusion Models, LLMs, Clustering, SVM, Random Forest.
- Python Tools & Modules: PyTorch, Tensorflow, Pandas, NumPy, Keras,, Sklearn, Seaborn, Matplotlib, SciPy.

Computer Enthusiast

- Scientific Programming: Python, bash, tcl/tk, slurm/pbs scripts.
- Highlighted Skills: AWS and HPC computing, GIT, DVC; Data Version Control (Iterative AI)
- Linux architecture (*Networking, Security and File server):* Admin role in troubleshooting system-related issues in PhD research group: Designed LDAP-based client-server protocol (400 TB file server+10 clients) •

Simulation Packages

- APIs: Atomic Simulation Environment (ASE), BioSimSpace, OpenMM, BioPython, MDTraj, AlphaFold
- Schrödinger Suite: Potentially explored backend workflow of various packages during the summer internship.
- Cheminformatics: OpeneyeKit, RDKit, OpenBabel, PaDel, Balloon, and Confab
- Simulation Packages: **MD:** NAMD, AMBER, DL-POLY, Gromacs, Desmond • **QM:** Siesta, Gaussian16, Orca, Terachem, GAMESS, VASP, USPEX, Quantum-Espresso • **Docking:** Autodock, Glide, Gold, OEDocking.
- Visualization: VMD, Pymol, Chimera, Molden, Gabedit, Gaussview, VESTA, Avogadro, Mercury.
- Biophysics skills: Protein purification, X-ray crystallography, and CyroEM

ORAL & POSTER PRESENTATIONS:

- Gupta, Aayush, Oral Presentation, ACS Meeting, San Francisco, USA. (Apr'17).
- Gupta, Aayush, Poster Presentation, "Modeling of CO_2 Reduction in Ionic Liquid Catalyzed 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 prestigious **Chancellor's Student Service and Leadership Award** at UIC, recognized twice for outstanding contributions *(Apr'20 & Apr'22)*
- Acknowledged with the Best TA Award for excellence in facilitating General Chemistry II Discussion & Lab (CHEM124/125) *(May'18)*
- Honored with the ***"GSC Travel Award"*** and ***"Student Presenter Award"*** at UIC for exemplary research and presentation skills. *(2017)*
- Organized "Chicago Biophysical Networking Event" at UIC, fostering connections among professionals in the field. (*Sep'19)*
- Actively served as a mentor at Science Club by Northwestern University, guiding and inspiring aspiring young minds.
- Invited as a panelist at the event ***"Graduate School Reality Check"*** event during the ACS meeting in San Francisco. (2017)
- Selected as one of the top invitees to attend the prestigious *"Indian Science Academies Workshop"* held at **BIT-Mesra**, Deoghar.
- Secured the esteemed 5top100 scholarship to conduct research at **MIPT, Moscow, Russia**. *(% intake : 5)*
- Awarded the highly competitive **Indian Academies of Sciences** - Summer Research Fellowship. *(% intake : 2)*
- Attained a **Diploma in Computer Application** (DCA) from a renowned Public University in India, achieving an A+ grade.
- Delivered an engaging and informative presentation on **"*Darwin Awards*"** at IGNITE, showcasing 20 slides in just 5 minutes, and invited as a speaker at the Freshers event at ICT.
- Avid Badminton player and Marathon Runner, and Poker champion at Schrödinger Poker Night.