Aayush Gupta

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SUMMARY

Innovation-driven computational chemist. Research interests involve integration of machine learning with next-generation quantum and classical molecular modeling. Versatile skills in computer programming, data science, and building Linux servers and GPUs. Strong experience in developing computational workflows for solving electronic structure and protein-drug modeling. Entrepreneurial plus independent research skills from framing new ideas, building prototypes to documenting in peer-reviewed journals (track record of first-author publications). Passionate about learning and implementing novel and challenging techniques that are advancing the science.

EDUCATION

University of Illinois at Chicago
- Ph.D. Candidate *(Computational Biophysics)* Aug'16 – Dec'21(Exp.)
  - Advisor: Prof. Huan-Xiang Zhou
- M.S. *(Chemistry)* *Aug'16 – Dec'18*

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

RESEARCH EXPERIENCE

PhD Research | UIC | *Advisor: Prof. Zhou* *Ongoing*
- 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 a 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: DFT modeling of electron transport in peptide helices subject to chirality induced spin selectivity (CISS) effect and its application in protein-protein association.

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 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'13*
- 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 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 and Zhou, Huan-Xiang. Artificial Intelligence Guided Conformational Sampling of Intrinsically Disordered Proteins. *Manuscript in preparation.*
2. Gupta, Aayush and Zhou, Huan-Xiang. (2021). Machine Learning-Enabled Pipeline for Large-Scale Virtual Drug Screening. *Journal of Chemical Information and Modeling* doi:10.1021/acs.jcim.1c00710 **[PDF]**
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 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]**
5. Gupta, Aayush, Oral Presentation, ACS Meeting, San Francisco, USA. (Apr'17).
6. 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

- Recipient of **Chancellor's Student Service and Leadership Award** at UIC *(Apr'20)*
- 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.