Azmine Toushik Wasi

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[Google Scholar](#) | [Semantic Scholar](#)| | [Kaggle](#)

SUMMARY

I am Azmine Toushik Wasi, an aspiring AI researcher and engineering student. My research focuses on exploring Graph Neural Networks (GNNs) in Biomedical AI, with an emphasis on structural biology, neuroscience, biomedical, and molecular domains. In addition to my GNN research, my other research interests include Natural Language Processing (NLP) and Human-Centered AI for interdisciplinary works. **I am looking forward to pursue a PhD in Fall 2025 to continue research.** My research has been published in prestigious venues such as COLING'24, ICLR'24 Tiny Papers Track, CSCW'24 Posters and workshops of NeurIPS'23, AAAI'24, ICML'24 and CHI'24. I am actively seeking research opportunities in theoretical or applied GNNs or any medical AI works. I am a quick learner and highly adaptable, capable of leading projects and teams. I enjoy exploring new topics, sharing knowledge, refining existing skills, experimenting with new techniques, and challenging my capabilities.

EDUCATION

Shahjalal University of Science and Technology — Sylhet, Bangladesh
Industrial and Production Engineering — *2020-Present*

- Expected to graduate in January 2025
- **Coursework related to ML:** MAT103G: Differential Calculus and Solid Geometry, MAT104G: Integral Calculus and Differential Equations, MAT207G: Vectors, Matrices and Laplace Transformation, CSE203G: Introduction to Computer Language, IPE251: Engineering Statistics, IPE321: Numerical Analysis, IPE339: Operations Research, IPE431: System Modeling and Simulation

Cumilla Shikkha Board Model College — Cumilla, Bangladesh
Higher Secondary Certificate in Science — *2017-2019*

- Won multiple regional and national Science Olympiads, including Chemistry (1st, regionally), Physics (5th, regionally), Earth Science (National Winner, joined national training camp), Zoology, and Programming (3rd, regionally).
- Advisor and Mentor, College Science Club and Olympiad Club

RESEARCH INTERESTS

- **Machine Learning (AI4Science)**: I am working on theoretical and applied machine learning, especially probabilistic modeling and inference, generative models, GFlowNets and its applications, etc.; broadly related to AI for Science. I aim to solve scientific problems in the medical sector (drugs and biomolecules), climate change, and manufacturing - industrial sectors (Digital Twins).
- **Bio-/Medical AI**: I am developing AI systems for Healthcare, focusing on Computational Molecular Biology - Neuroscience, Bioinformatics, Computational Drug Discovery (CADGL), molecular properties prediction, protein discovery, binder design and binding affinity, molecular interactions and affinity, structural biology, and healthcare optimization (Glucose control (ICLR'24)). I have experience with de novo protein generation (RFDiffusion, FoldFlow, Croma, etc.) models and RL-inspired/energy-guided geometric/sequential structural biology (Proteins, RNA, Genome & Drugs) modeling tools with GNNs, Flow Matching, GFlowNets, and Diffusion models. Additionally, I have experience in computational neuroscience.
- **Graph Neural Networks (GNN)**: I am exploring Graph Neural Network or Geometric Machine Learning Theories, applying and improving GNN models and resources in Healthcare (Drug Discovery, Interactions, Protein Design & Binding, and Micro/Macro-Molecules) (DDI), Knowledge Graphs (BanglaAutoKG (COLING'24) and HRGraph (ACL'24W)), Supply Chains (SupplyGraph (AAAI'24W)), and spatial modeling (ClimateAI).

- **Human-Centered AI (HAI)**: Despite extensive coursework in ergonomics, Human Factors Engineering (HFE), behavior studies, and psychology within our IPE curriculum, there is a notable gap in inter-disciplinary research between IPE and AI in Bangladesh. Motivated by this, I am integrating HFE (Ownership, Individuality in AI (CHI'24W); Ergonomics in LLMs (ICML'24-W), Religious/Cultural Bias (CSCW'24, CHI'24W; EMNLP'25-InReview), Fairness and Reliability (ARBEx, Social Biases (CHI'24W)) into AI systems, focusing on AI perspectives of IPE.
- **Natural Language Processing (NLP)**: I am developing Knowledge Graphs (COLING'24) and Bangla Knowledge Systems; motivated by NLP + GNNs. I am also working on interdisciplinary CSS, Climate NLP, Human-centric NLP (Ownership & Individuality in LLM content generation (CHI'24W); Ergonomics in LLMs (ICML'24-W), Bias in LLMs (CSCW'24, CHI'24W; EMNLP'25-InReview)), ChemicalLMs, and BioMedNLP (Molecules+NLP (ICLR'24)).

Research Experience

Visitng Researcher   October, 2022 - Present
Data Intelligence Lab, Hanyang University   *Part time, Remote*
- I am working on Graph Neural Networks (Theoretical GNNs, Knowledge Graphs and Bangla NLP, Applications in Healthcare domain), Medical AI, and Human-centric aspects of LLMs; supervised by Prof. Dong-Kyu Chae, and mentored by Taki Hasan Rafi.
- **Accepted Works:** Bangla KG Construction (LREC-COLING'24), Molecule Classification by NLP (ICLR'24 Tiny Papers Track), Dialects in AI Spaces (CSCW'24 Posters), HCI+LLM Evaluation (CHI2024W).
- **Works in Review:** Reliable Facial Emotion Recognition (ACCV'24), Drug Discovery (TCBB), Auditing Bias in LLMs (EMNLP'24), GNN Enhancement, SMART App for Legal Documents, and Cognitive Ergonomics in UI Design.

Student Research Assistant   July, 2024 - Present
Mila - Quebec AI Institute   *Remote*
- My research centers on geometric and sequential structural biology (focusing on proteins, RNA, genomes, and drugs), and multi-modal alignment problems. I use GNNs, Flow Matching, GFlowNets, and Diffusion models to model these, with an emphasis on RL-inspired and energy-guided approaches. Additionally, I work on de novo protein generation models such as RFDiffusion, FoldFlow, and Croma.
- Currently, I collaborate on similar projects with Mila alumni, current students, and academics. I am directly mentored by Riashat Islam (PhD, McGill and Mila; RS at SDAIA/NCAI; Ex-RS at DreamFold AI, a Mila startup).

Student Researcher   2022 - Present
Shahjalal University of Science and Technology   *Part time, Remote*
- Founded Computational Intelligence and Operations Lab - CIOL, SUST to accelerate IPE + ML combinational research through guiding and mentoring aspiring researchers.
- I am collaborating with Prof. Manjurul Ahsan (University of Oklahoma) and Prof. Mahathir M Bappy (Louisiana State University) on GNNs, Digital Twins, Advanced manufacturing, and Medical AI applications.
- **Works:** Decision-focused Inventory Routing (NeurIPS'23W), Hate Speech Detection and XAI (NeurIPS'23W), Supply Chain Graph Dataset (AAAI'24W), Glucose Level Control System (ICLR'24 Tiny Papers Track), 2 papers on Dark sides of LLM-assisted Writing (In2Writing, CHI2024W), Human-centered LLM Evaluation (HEAL, CHI2024W), Cognitive Ergonomics in LLM (ICML'24W), HR Knowledge Graph (ACL'24W).

Selected Publications

AI4Science, GNNs and Medical AI:

- **BanglaAutoKG: Automatic Bangla Knowledge Graph Construction with Semantic Neural Graph Filtering** | Accepted | LREC-COLING'24 | ACL Anthology | arXiv | GitHub
  Azmine Toushik Wasi, Taki Hasan Rafi, Raima Islam, Dong-Kyu Chae

- **Neural Control System for Continuous Glucose Monitoring and Maintenance**
  Accepted | ICLR'24 Tiny Paper Track | OpenReview | arXiv | GitHub
  Azmine Toushik Wasi

- **When SMILES have Language: Drug Classification using Text Classification Methods on Drug SMILES Strings** | Accepted | ICLR'24 Tiny Paper Track | OpenReview | arXiv | GitHub
  Azmine Toushik Wasi, Karlo Serbetar, Raima Islam, Taki Hasan Rafi, Dong-Kyu Chae

- **SupplyGraph: A Benchmark Dataset for Supply Chain Planning using Graph Neural Networks**
  Accepted | AAAI'24 - GCLR Workshop | arXiv
  Azmine Toushik Wasi, MD Shafikul Islam Sohan, Adipto Raihan Akib

- **HRGraph: Leveraging LLMs for HR Data Knowledge Graphs with Information Propagation-based Job Recommendation**
  Accepted | ACL'24 - Knowledge Graphs and LLMs Workshop
  Azmine Toushik Wasi

- **Optimizing Inventory Routing: A Decision-Focused Learning Approach using Neural Networks**
  Accepted | NeurIPS'23 - New in ML Workshop | arXiv
  MD Shafikul Islam Sohan, Azmine Toushik Wasi

Human-centric AI:

- **DiaFrame: A Framework for Understanding Bengali Dialects in Human-AI Collaborative Creative Writing Spaces**
  Accepted | CSCW'24 Posters Track
  Azmine Toushik Wasi, Taki Hasan Rafi, Dong-Kyu Chae

- **Exploring Large Language Model Systems Design Perspective Using Cognitive Ergonomics**
  Accepted | ICML'24 - LLMs and Cognition Workshop | arXiv
  Azmine Toushik Wasi

- **LLMs as Writing Assistants: Exploring Perspectives on Sense of Ownership and Reasoning**
  Accepted | CHI'24 - In2Writing Workshop | arXiv
  Azmine Toushik Wasi, Mst Rafia Islam, Raima Islam

- **Ink and Individuality: Crafting a Personalised Narrative in the Age of LLMs**
  Accepted | CHI'24 - In2Writing Workshop | arXiv
  Azmine Toushik Wasi, Raima Islam, Mst Rafia Islam

- **Exploring Bengali Religious Dialect Biases in Large Language Models with Evaluation Perspectives**
  Accepted | CHI'24 - HEAL Workshop | arXiv
  Azmine Toushik Wasi, Raima Islam, Mst Rafia Islam, Taki Hasan Rafi, Dong-Kyu Chae

In-Progress Studies and Review Submissions

AI4Science, GNNs and Medical AI:

- **Attentive Feature Extraction with Reliability Balancing for Robust Facial Expression Learning**
  In Review | ACCV'24 | arXiv
  Azmine Toushik Wasi, Taki Hasan Rafi, Raima Islam, Karlo Serbetar, Dong-Kyu Chae

- **CADGL: Context-Aware Deep Graph Learning for Predicting Drug-Drug Interactions**
  In Review | IEEE/ACM Transactions on Computational Biology and Bioinformatics | arXiv
  Azmine Toushik Wasi, Taki Hasan Rafi, Raima Islam, Karlo Serbetar, Dong-Kyu Chae

- **Gaussian Regularization in Neural Graph Learning**
  In Review
  Azmine Toushik Wasi, Taki Hasan Rafi, Dong-Kyu Chae

Human-centric AI:

- **Interpreting and Eliminating Bangla Cultural Dialect Bias in LLMs**
  In Review | ACL-ARR | Received 4/5 in ARR April Meta-Review
  Azmine Toushik Wasi, Raima Islam, Mst Rafia Islam, Farig Sadeque, Taki Hasan Rafi, Dong-Kyu Chae

- **LegalMind: An Intelligent Mobile App for Legal Document Reading with Smart Entity Mapping and Question Answering**
  In Review
  Azmine Toushik Wasi, Mst Rafia Islam, Taki Hasan Rafi, Dong-Kyu Chae

- **Exploring Cognitive Ergonomics Principles to Improve UI Design**
  In Review
  Azmine Toushik Wasi, Yeamim Touhid, Taki Hasan Rafi, Dong-Kyu Chae

TECHNICAL SKILLS

- **Languages**: Python (Advanced), C, C++, MATLAB, R, SQL
- **DS & ML Tools (Python)**: NumPy, Pandas, Matplotlib, Seaborn, Scikitlearn, Tensorflow, PyTorch
- **Machine Learning Technique**: Statistical ML Methods, Deep Learning, Graph Neural Networks, GFlowNets, Computer Vision, Explainable AI, Robust Modeling, etc
- **Data Science Techniques**: EDA, Experimental Design, Hypothesis Testing, Sampling and Decision making
- **Computational Biology and Bio-molecules**: Molecular Networks, Classification, Molecular Interaction Detection and Classification, Generative Modeling with Flow Matching, Graph Diffusion, and Energy-guided molecule generation
- **Human-centered AI**: LLM Customization, Survey Design, UI/Framework Design and Development, Data Collection and Analysis
- **Others**: GitHub, Collaborative tools (Replit, Colab, and Kaggle), Parallel and Distributed Computing

REVIEWING SERVICES

- **Conference or Journal Reviewer**
  - **AI/ML**: ICLR Tiny Papers Track (2024).
  - **NLP**: ACL ARR February, April, June 2024 [View in official reviewer list].
  - **HCI/HAI**: CSCW 2024, UbiComp/ISWC 2024, IDC 2024.
  - **Journals**: Complex & Intelligent Systems [Impact factor 5.8 (2022)].
  - Total conference or journal paper reviewed: 32
- **Workshop Program Committee and Reviewer**
  - **ICML 2024**: AI4Science, Large Language Models and Cognition
  - **ACL 2024**: TextGraphs-17, ClimateNLP, SMM4H, Language + Molecules, KALLM (KG+LLMs), WASSA
  - **MICCAI 2024**: GRaphs in biomedicAl Image anaLysis, Fairness in Medical Imaging,
  - Total top conference workshop paper reviewed: 27

ACHIEVEMENTS

- Winner at ACL'24: #SMM4H Workshop - Shared task 3.
- Received **ICLR 2024 Travel Award**, along with complimentary in-person full conference registration.
- **Finalist (Top 4)** of ProcessMiner QCRE Data Challenge, **IISE Global Conference and Expo, 2023** — Report
- **Kaggle Notebooks Grandmaster** (Highest Rank: 36th globally) Datasets & Discussions Master

- GDN Presenta - Champion | Podiam 1.0 - 2nd Runners Up
- National High School Programming Contest 2016 , 2017 – Regional Winner; National Top 30 in both
- Inter School & College Programming Contest 2019 – Regional(3rd)- National Top 30
- National Earth Science Olympiad 2019 – National Winner
- National Chemistry Olympiad 2019 – 1st (Regional)
- National Physics Olympiad 2019 – 5th (Regional)
- The Queens Commonwealth Essay competition 2019 – Silver Award

Projects and Tutorial Blogs

- **ML Learning Hub: Online ML University** | GitHub [around 100 stars]
  A curated list of FREE courses available online from top universities of the world on CS-DS-ML.
- **Paper Reviews, Organization and Collection**
  Awesome ICML 2024 Graph Paper Collection (GitHub) [95+ stars]
  Awesome ICLR 2024 Graph Paper Collection (GitHub) [50+ stars]
  Awesome ICLR 2024 LLM Paper Collection (GitHub) [20+ stars]
- **Bias-Variance Tradeoff —Tutorial with NumPy & Seaborn** | Kaggle
  A brief tutoial on Bias-Variance Tradeoff. Used pandas, numpy, seaborn, Scikitlearn.
- **Divorce Prediction & Reasons : Machine Interpretation Analysis with XGB, SHAP, RFE** | Kaggle | **Kaggle XAI Spotlight Newsletter**
  A detailed exploratory data analysis of Divorce with necessaey Viz. Predicted with XGBoost. Then, analyzed featured for PCA. Used pandas, numpy, seaborn, xgboost, shap, scikit-learn.
- **Time Series Analysis and Forecasting** | Kaggle
  A detailed blog tutorial on different time series analysis methods and examples.

Work Experience

Project Executive March, 2022 – October, 2023
10 Minute School *Part time, Hybrid*

- Developed 30+ Automation tools for content development and quality control automation using Python & ML (NLP, CV) Techniques, increasing productivity and quality by 500%-1000%.
- Developed and maintained 180+ interconnected google sheets for multiple projects | Developed 22K+ educational and promotional contents.
- Worked in 50+ different projects | Led 35+ project segments. Led and managed 04 teams with 15+ individuals in different projects for 1 year.

Live-Class Team Resource Executive September, 2021 – February, 2022
Shikho Technologies *Part time, Remote*

- Created and quality assured over 480 educational materials

Manager of Research and Development 2021-2023
BasaKhujo *Self Employed, Remote*

- Mangaged in product research, market analysis, product development, and deployment, while also contributing to analytics refinement and growth monitoring with optimized metrics for cross-validation.

Training Programs

Computational Neuroscience Summer School July 2024
Neuromatch Academy *Remote*

- This curriculum emphasizes code-first, hands-on learning by integrating machine learning and causality research into neuroscience modeling. It covers basic to advanced modeling techniques, including machine learning, deep learning, biologically plausible dynamical systems, stochastic processes, measurement insights, and methods for dynamic system control using optimal control and reinforcement learning.
- My pod project focused on brain actvity analysis with machine learning on fMRI data.

CCAI Summer School 2024 Jun-Aug 2024
Climate Change AI *Remote*

- After completing the program, I will gain practical experience in applying AI to various climate-related fields and developed a good understanding of the ethical, regulatory, and environmental implications of AI technology in addressing climate challenges.

Aspire Leaders Program 2023   Apr-Sept 2023

Aspire Institute Inc., Harvard university   *Remote*

- Participated in a rigorous leadership development program at one of the world's most prestigious universities, gaining invaluable skills and knowledge in areas such as decision-making, strategic planning, team management, communication, conflict resolution, project management, and cross-functional collaboration through participation in various program activities and projects.

OTHER TECHNICAL AND SOFT SKILLS

- **Office Suites:** MS Word, MS PowerPoint, MS Excel, Google G-Suite
- **Writing Skills:** Creative Writing, Technical Writing, Copywriting, SEO
- **Design and Multimedia:** Adobe Illustrator, Adobe Photoshop, Video Editing
- **Soft Skills:** Creativity, Management, Communication, Teamwork, Decision Making, Conflict Resolution, Delegation, Motivation, Communication, Team Building, Time Management, Goal Setting, Coaching, Collaboration, Problem Solving, Adaptability, Emotional Intelligence

ORGANIZATIONAL/VOLUNTARY EXPERIENCE

- **Founder and Director** at *Computational Intelligence and Operations Lab – CIOL* (2022 - Present)
  - I founded CIOL to accelerate IPE-AI collaborative research at SUST-IPE, filling up the current gap of ML-focused research in the department. Collaborating with our seniors, we ensure that the lab is well-equipped with the necessary resources and expertise; and actively involved in different research projects.
- **Product Tester** at *DeepLearning.AI* (May 2023 - December 2023)
  - Testing DeepLearning.AI courses on Coursera, providing suggestions for improvement.
  - Worked on Probability & Statistics for Machine Learning and Data Science course of Mathematics for Machine Learning Specialization, by Luis Serrano on Coursera. (Acknowledgement)
- **Pie & Ai Ambassador** at *DeepLearning.AI* (October 2022 - December 2023)
  - Arranged and took several workshop and meetups.
  - Trained Python and latest ML Technologies over 300+ individuals from different background.
- **Wing Director, Technical Facilities Enhancement** at *Black Brains* (Sept. 2021 - Jan. 2022)
  Executive Officer (Technology, Curriculum, and Research) at *Black Brains* (Joined Nov 15, 2020)
  - Development of Black Brains Office Assistant App.
  - Developing Black Brains Micro-courses (Curriculum, Content Design, Course Assessments Design, App Integration, Database and Overall administration)
  - Database design and management. Regular technical research, analysis and development. Website & App maintainance.
- **Information Technology Manager** at *Bangladesh Youngster Social Organisation* (Jan 2019 - Oct 2021)
  - Managing Program-related IT Support stuffs and tasks
  - BYSO - App Development for android platform with Top #3 ranking in communications app in PlayStore. Created Central Database, and necessary management tools. Developed IT Structure for the organization and increased productivity.
- **Judge** at *The Queen's Commonwealth Essay Competition 2021* (July 2021)
  - The QCEC is the world's oldest international writing competition for schools, established in 1883. This year QCEC received about 26,000 submissions from all the commonwealth countries.
- **Feature Writer & Content Developer** at *Tachyon* (June 2021 - 2022)
  - Wrote several features on programming, data science, and Machine Learning. Also, developed several visual contents on different programming topics. URL: https://tachyonts.com/
- **Online Volunteer** at *United Nations Volunteers* (July 2020 - April 2021)
  - Supporting in many roles as Content Writer, Graphics Designer, Translator etc in various projects.
- **C Programming Mentor** at *IPSC Programming Club* (2016-2017)
  - Trained aspiring programmers of the club for National High School Programming Contest.

Talks and Training Workshops Taken

- **Pie & AI: Sylhet - ML Research for Engineering Undergrads: A Pathway** | Oct 23, 2023 | Workshop
- **Introduction to Research (IPE and ML Focused)** | Sept 8, 2023 | Workshop
- **Navigating the Digital Frontier | Building the Basics on ML and AI** | Aug 25, 2023 | Guest Talk
- **Building AI and Machine Learning Model: How to Start?** | Jul 23, 2023 | Workshop
- **Pie & AI: Sylhet - Use of ChatGPT and Generative AIs** | Mar 3, 2023 | Guest Lecture
- **Pie & AI: Sylhet – Machine Learning for Engineering Students** | Jan 25, 2023 | Talk
- **Pie & AI: Sylhet - Introduction to Python for AI** | Oct 15-22, 2023 | Workshop

Learning and Certifications

Forage - Virtual Interships
Data@ANZ Program - ANZ, Open-Access Data Science & Advanced Analytics Virtual Experience Program - BCG, Careers in Tech Program - Commonwealth Bank, Engineering: Undergraduate & Masters Asia Virtual Experience Program, Digital Technology Data Analytics Program - General Electric, Engineering Virtual Program - Goldman Sachs

Google Career Certificates (Coursera)
Data Analyst, Advanced Data Analyst, BI Analyst, IT Automation with Python, IT Support Professional, Project Management

DataCamp Learning Paths
Career Tracks: Python Programmer, Machine Learning Scientist with Python, Data Analyst with Python, Data Scientist with Python

Coursera Specializations
Machine Learning Specialization, Deep Learning Specialization, Natural Language Processing Specialization, TensorFlow: Advanced Techniques Specialization, Generative Adversarial Networks (GANs) Specialization - from DeepLearning.ai; Python for Everybody, Data Science Fundamentals, Python 3 Programming, Applied Data Science with Python, Supply Chain Management, Project Management Principles and Practices

Reference

Dong Kyu Chae (**dongkyu@hanyang.ac.kr**)
Assistant Professor, Department of Computer Science at Hanyang University (Sep'20 – Present)

Riashat Islam (**riashat.islam.93@gmail.com**)
Senior Research Scientist, SDAIA/NCAI (Jul'24 - Present); Ex-RS, DreamFold AI (a Mila based startup); PhD, McGill University with Mila - Quebec AI Institute (2017 - 2023)

Mahathir Mohammad Bappy (**mmbappy@lsu.edu**)
Assistant Professor, Louisiana State University (2024 - Present)

Md Manjurul Ahsan (**mdmanjurulahsan@gmail.com**)
Research Assistant Professor, University of Oklahoma (2024 - Present)

Taki Hasan Rafi (**takihr@hanyang.ac.kr**)
PhD Student, Hanyang University (Jan'22 – Present)