

# Md Hossain Shuvo, Ph.D.

## Assistant Professor

Department of Computer Science  
Prairie View A&M University  
Prairie View, TX USA

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## EDUCATION

**DEC 2023**

**Virginia Tech**  
Ph.D. in Computer Science  
**Advisor:** Dr. Debswapna Bhattacharya  
GPA: 3.88/4.0

**JUL 2017**

**Alabama A&M University**  
M.Sc. in Computer Science  
**Advisor:** Dr. Yujian Fu  
GPA: 4.0/4.0

**JUL 2014**

**Bangladesh University of Business and Technology**  
B.Sc. in Computer Science  
**Advisor:** Mr. Md Saifur Rahman  
CGPA: 3.86/4.0

## RESEARCH INTERESTS

Computational Biology  
Machine Learning  
Data Analytics  
Artificial Intelligence

## RESEARCH EXPERIENCE

**AUG 2021 – DEC 2023**

**Virginia Tech**  
**Advisor:** Dr. Debswapna Bhattacharya  
**Research direction:** application of machine learning in developing computational methods for addressing problems related to protein complexes

**JAN 2018 – JUL 2021**

**Auburn University**  
**Advisor:** Dr. Debswapna Bhattacharya

**AUG 2015 – JUL 2017**

**Research direction:** application of machine learning in developing computational methods for addressing problems related to protein structure prediction

**Alabama A&M University**

**Advisor:** Dr. Yujian Fu

**Research direction:** development of tools for analyzing interactive behaviors in embedded and heterogeneous robotic systems

## ACADEMIC EXPERIENCE

**JAN 2024 - PRESENT**

**Prairie View A&M University**

**Position:** Assistant Professor, Dept. of CS

**AUG 2018 – JAN 2020**

**Auburn University**

**Position:** Graduate Teaching Assistant, Dept of CSSE

**Courses:**

1. **COMP 5970/6970:** Computational Biology
2. **COMP1210:** Fundamental of Computing I

**MAY 2016 – JUL 2016**

**North Alabama Center for Educational Excellence (NACEE)**

**Position:** Assistant Mentor

**Topic:** implementing multi-tasking and interactive behavior in NAO Humanoid robot

**JAN 2015 – JUL 2015**

**Dhaka Commerce College, Dhaka, Bangladesh**

**Position:** Lecturer, Dept. of Stat, Math and COMP

**JAN 2014 – DEC 2014**

**Dhaka Cambrian College, Dhaka, Bangladesh**

**Position:** Lecturer, Dept. of Information and Communication Technology

## REFEREED PUBLICATIONS

**2025**

18. **M. H. Shuvo**, D. Bhattacharya. EquiRank: improved protein-protein interface quality estimation using protein-language-model-informed equivariant graph neural networks International Conference on Intelligent Biology and Medicine, 2024 Computational and Structural Biotechnology Journal, Volume 27, 160 - 170, 2025

**2024**

17. R. Roche, B. Moussad, **M. H. Shuvo**, S. Tarafder, D. Bhattacharya, EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks. *Nucleic Acids Research*, 2024 gkae039, 10.1093/nar/gkae039

**2023**

16. **M. H. Shuvo**, M. Karim, R. Roche, and D. Bhattacharya, "PIQLE: protein-protein interface quality estimation by deep graph learning of multimeric interaction geometries", *Bioinformatics Advances*, 2023, vbad070, 10.1093/bioadv070.
15. **M. H. Shuvo**, M. Karim, and D. Bhattacharya, "iQDeep: an integrated web server for protein scoring using multiscale deep learning models", *Journal of Molecular Biology*, 168057, 2023. doi: 10.1016/j.jmb.2023.168057
14. R. Roche, B. Moussad, **M. H. Shuvo**, D. Bhattacharya, "E(3) equivariant graph neural networks for robust and accurate protein-protein interaction site prediction", *PLOS Computational Biology*, 19, e1011435, doi: 10.1371/journal.pcbi.1011435
13. S. Bhattacharya, R. Roche, **M. H. Shuvo**, and D. Bhattacharya, "Contact-assisted threading in low-homology protein modeling", *Methods in Molecular Biology book series*, vol. 2627, 2023, doi: 10.1007/978-1-0716-2974-1\_3

## 2022

12. R. Roche, S. Bhattacharya, **M. H. Shuvo**, and D. Bhattacharya, "rrQNet: Protein contact map quality estimation by deep evolutionary reconciliation", *Proteins*, Jun 2022, doi: 10.1002/prot.26394.

## 2021

11. **M. H. Shuvo**, M. Gulfam, and D. Bhattacharya, "DeepRefiner: high-accuracy protein structure refinement by deep network calibration", *Nucleic Acids Research*, vol. 49, no. W1, pp. W147–W152, Jul. 2021, doi: 10.1093/nar/gkab361
10. S. Bhattacharya, R. Roche, **M. H. Shuvo**, and D. Bhattacharya, "Recent Advances in Protein Homology Detection Propelled by Inter-Residue Interaction Map Threading", *Front Mol Biosci*, vol. 8, p. 643752, 2021, doi: 10.3389/fmolb.2021.643752.
9. A. Kryshtafovych, . . . , **M. H. Shuvo**, . . . , "Modeling SARS-CoV-2 proteins in the CASP-commons experiment", *Proteins*, vol. 89, no. 12, pp. 1987–1996, Dec. 2021, doi: 10.1002/prot.26231.

## 2020

8. **M. H. Shuvo**, S. Bhattacharya, and D. Bhattacharya, "QDeep: distance-based protein model quality estimation by residue-level ensemble error classifications using stacked deep residual neural networks", *Bioinformatics*, vol. 36, no. Suppl 1, pp. i285–i291, Jul. 2020, doi: 10.1093/bioinformatics/btaa455
7. R. Alapati, **M. H. Shuvo**, and D. Bhattacharya, "SPECS: Integration of side-chain orientation and global distance-based measures for improved evaluation of protein structural models", *PLoS One*, vol. 15, no. 2, p. e0228245, 2020, doi: 10.1371/journal.pone.0228245

## 2016

6. **M.H. Shuvo**, Y. Fu, "Sonar sensor virtualization for object detection and localization", *SoutheastCon 2016*, 1–8. doi: 10.1109/SECON.2016.7506699
5. Y. Fu, **M.H. Shuvo**, "An approach to analyzing adaptive intelligent vehicle system using SMT solver", In *2016 International Conference on Control, Decision and Information Technologies*, (CoDIT)., pp. 313–319, doi: 10.1109/CoDIT.2016.7593580
4. Y. Fu, **M.H. Shuvo**, "Android-Based Remote Robot Control System". In, *2016 ASEE Annual Conference & Exposition Proceedings*. ASEE Conferences, New Orleans, Louisiana, p.26251, doi: 10.18260/p.26251

## 2015

3. S. Rahman, **M.H. Shuvo**, "Advancement of Information System in the Health Sphere in Rural-Urban Areas of Developing Countries: A Case Study of Bangladesh". IJIRSET, Vol. 4, Issue 6, June 2015, doi: 10.15680/IJIRSET.2015.0406131
2. **M.H. Shuvo**, T. Haque, "Suspicious Behavior Detection Framework for Social Networking Sites Using Hidden Markov Model", 2015 Dhaka Commerce College Journal, Vol 7, Issue 1, P. 173 – 192

## 2014

1. M.M. Rahman, S. Ahmed, **M.H. Shuvo**, "Nearest Neighbor Classifier Method for Making Loan Decision in Commercial Bank". IJISA, 6, 60–68, doi: 10.5815/ijisa.2014.08.07

## ABSTRACTS AND POSTERS

### Abstracts

9. **M. H. Shuvo**, M. Karim, and D. Bhattacharya, "Protein modeling and accuracy estimation by Bhattacharya group in CASP15," CASP15 abstract, p. 35, 2022.
8. **M. H. Shuvo**, M. Gulfam, and D. Bhattacharya, "Deep network calibration for protein structure refinement," 13th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics, ACM-BCB 2022.
7. **M. H. Shuvo**, S. Bhattacharya, R. Roche, and D. Bhattacharya, "Protein tertiary structure prediction by Bhattacharya group in CASP14," CASP14 abstract, p. 38, 2020.
6. **M. H. Shuvo**, and D. Bhattacharya, "Protein model accuracy estimation by Bhattacharya groups in CASP14," CASP14 abstract, p. 39, 2020.
5. **M. H. Shuvo**, and D. Bhattacharya, "Protein structure refinement by Bhattacharya groups in CASP14," CASP14 abstract, pp. 40–41, 2020.
4. D. Bhattacharya, R. Alapati, and **M. H. Shuvo**, "Protein structure prediction and refinement by Bhattacharya human group in CASP13," CASP13 abstract, pp. 29-30, 2018.
3. R. Alapati, **M. H. Shuvo**, and D. Bhattacharya, "clustQ: Multi-model QA using superposition-free weighted internal distance comparisons," CASP13 abstract, p. 31, 2018
2. D. Bhattacharya and **M. H. Shuvo**, "refineD: Protein structure refinement using machine learning guided restrained relaxation," CASP13 abstract, p. 32, 2018
1. D. Bhattacharya and **M. H. Shuvo**, "scoreD: Estimating Global Distance Test using deep discriminative binary classifier ensemble," CASP13 abstract, p. 33

### Posters

3. **M. H. Shuvo**, D. Bhattacharya. "EquiRank: improved protein-protein interface quality estimation using protein-language-model-informed equivariant graph neural networks", PVAMU R&I Week, 2024
2. S. Adepoju, **M.H. Shuvo**, "How Machine Learning Can Revolutionize Building Comfort: Unveiling the Impact of Occupancy Prediction Models on HVAC Control System of the Roy G. Perry College of Engineering Building", PVAMU R&I Week, 2024
1. **M. H. Shuvo**, S. Bhattacharya, D. Bhattacharya, "QDeep: distance-based protein model quality estimation by residue-level ensemble error classifications using stacked deep residual neural networks", ISMB 2020

## PARTICIPATION IN COMMUNITY-WIDE ASSESSMENT

APR 2022 – AUG 2022	<b>15<sup>th</sup> Critical Assessment of Protein Structure Prediction (CASP15) challenge</b> <b>Role:</b> method development, technical support for double-blind testing of our developed methods in both server and human pipelines
MAY 2020 – SEP 2020	<b>14<sup>th</sup> Critical Assessment of Protein Structure Prediction (CASP14) challenge</b> <b>Role:</b> method development, technical support for double-blind testing of our developed methods in both server and human pipelines
APR 2020	<b>CASP Commons (COVID-19, 2020), a collaborative initiative for modeling the SARS-2-CoV structure</b> <b>Role:</b> Provided technical support for testing our developed methods in predicting and assessing SARS-2-CoV target
MAY 2018 – AUG 2018	<b>13<sup>th</sup> Critical Assessment of Protein Structure Prediction (CASP13) challenge</b> <b>Role:</b> method development, technical support for double-blind testing of our developed methods in both server and human pipelines

## HONORS AND AWARDS

Quantum Workshop Travel Fellowship	By the University of Tennessee at Chattanooga
Google Cloud Research Resource	\$5,000 resource credit by Google
The PHIT Workforce Development Program Grant [Co-PI]	\$432,078 by the University of Texas Health Science Center at Houston
GenAI Faculty Summit Travel Fellowship	Awarded by Google
FACULTY ENHANCEMENT PROGRAM	Awarded by the Roy G. Perry College of Engineering at PVAMU
NSF NDSA PFx instructor	Selected to be a PFx instructor
NSF NDSA RESEARCH AFFINITY COHORT	Selected as 1 of the 20 researchers
GOOGLE TEC EQUITY IMPACT FUND	\$50,000 non-dilutive funding, led jointly with Dr. Wang at PVAMU
ACCESS ALLOCATIONS	Principal Investigator (PI), NSF - XSEDE Research Allocation
PRATT FELLOWSHIP AWARD	Awarded Pratt Fellowship at Virginia Tech, 2023
YOUNG SCIENTIST EXCELLENCE AWARDS	Awarded 1 <sup>st</sup> place prize at 18 <sup>th</sup> annual MCBIOS conference, 2022
CONFERENCE FELLOWSHIP	I. Received fellowship award for MCBIOS 2022

**PUBLICATION RECOGNITION****TRAVEL FELLOWSHIP****POSTER AWARD**

II. Received ISMB 2020 fellowship award

DeepRefiner paper accepted for ACM-BCB 2022 Highlights track

Received travel grant for IEEE SoutheastCon 2016

Awarded 2<sup>nd</sup> place prize at AAMU STEM Day 2016

**SCIENTIFIC SOFTWARE DEVELOPMENT****EquiRank**

pLM-based Protein-protein interface quality estimation method  
[\[GitHub\]](#)

**PIQLE**

Protein-protein interface quality estimation method [\[GitHub\]](#)

**iQDeep**

Integrated protein scoring server [\[Server\]](#)

**DeepRefiner**

High-accuracy protein structure refinement server [\[Server\]](#)

**QDeep**

Single-model protein quality estimation method [\[GitHub\]](#)

**SPECS**

Improved evaluation method for protein structures [\[GitHub\]](#)

**EquiPPIS**

E(3) equivariant graph neural networks for robust and accurate protein-protein interaction site prediction [\[GitHub\]](#)

**EquiPNAS**

EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks [\[GitHub\]](#)

**rrQNet**

Protein contact map evaluation method [\[Github\]](#)

**TECHNICAL SKILLS****PROGRAMMING SKILLS**

Python, R, Java, C, C++, PHP, ASP, Apache Cordova MySQL, MSSQL

**APP DEVELOPMENT**

- I. Standalone application development with Java EE
- II. Mobile applications development in both Android and iOS
- III. Platforms Web applications development
- IV. Robotic applications development for EV3, NAO, and UAV

**SERVICES AND OUTREACH**

**COMPUTER SCIENCE CURRICULUM DEVELOPMENT COMMITTEE** Serving as a member of the CS Undergraduate Curriculum Development Committee

**COLLEGE OF ENGINEERING CURRICULUM DEVELOPMENT COMMITTEE** Served as a member of the COE Undergraduate Curriculum Development Committee

**DIVISION OF RESEARCH AND INNOVATION COMMITTEE** Serving as a member of the Division of Research and Innovation Committee for Computer Science at PVAMU

**FACULTY SEARCH COMMITTEE** Served as a member of the PVAMU faculty search committee

**REVIEWER** Served as a sub-reviewer for Bioinformatics, BIOKDD 2021, 2023, 2024, IEEE ACM/Transaction, IEEE CogMI and others

**EVENT MANAGEMENT**

- i. Provided logistic support on E-day 2020 at Auburn University
- ii. Provided logistic support on AAMU Senior High School Day 2016

**TECHNICAL COMMITTEE MEMBER**

Provided technical support by developing the complete submission management system for AAMU STEM Day 2016