Amarda Shehu

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EMPLOYMENT

University-wide Leadership — George Mason University

Inaugural Vice President and Chief AI Officer	August 2024 – present
Member, President's Executive Council	September 2025 – present

College of Engineering and Computing — Leadership Roles

Associate Dean for Research, College of Engineering and Computing	April 2025 – present
Academic Chair, AI-in-Gov Council, College of Engineering and Computing	January 2025 – present
Associate Dean for AI Innovation, College of Engineering and Computing	July 2023 – December 2024

Institute & Cross-Unit Leadership — George Mason University

Associate Vice President of Research, Institute for Digital InnovAtion	May 2022 – August 2024
Co-Director, Center for AI Innovation & Economic Competitiveness	August 2024 – present
Inaugural Founding Co-Director, Center of Excellence in Government Cybersecurity Risk Management and Resilience (crc.gmu.edu)	May 2023 – August 2024
Inaugural Founding Co-Director, Provost Transdisciplinary Center for Advancing Human-Machine Partnerships (cahmp.gmu.edu)	August 2019 – May 2022

Academic Appointments — George Mason University

Professor, Department of Computer Science	August 2018 – present
Associate Professor, Department of Computer Science	August 2014 – August 2018
Assistant Professor, Department of Computer Science	August 2008 – 2014
Affiliate Faculty, School of Systems Biology	August 2008 – present
Affiliate Faculty, Department of Bioengineering	August 2011 – present

Federal Appointment — National Science Foundation

Program Director (IPA), Information Integration and Informatics (III), Division of Information and Intelligent Systems (IIS), CISE Directorate	August 2019 – May 2022

EDUCATION

Doctor of Philosophy — Rice University, Houston, TX

Ph.D. in Computer Science	December 2004 – July 2008

Dissertation: *"Molecules in Motion: Computing Structural Flexibility"*
Committee: Kavraki LE (dissertation director), Vardi M, Clementi C, Nakhleh L

Master of Science — Rice University, Houston, TX

M.S. in Computer Science	August 2002 – December 2004

Thesis: *"Sampling Biomolecular Conformations with Spatial and Energetic Constraints"*
Committee: Kavraki LE (thesis director), Goldman R, Clementi C, Nakhleh L

Bachelor of Science — Clarkson University, Potsdam, NY

B.S. in Computer Science and Mathematics, *Summa Cum Laude*	January 2000 – May 2002

Honors Thesis: *"Structural and Computational Complexity Results on Testing Dimension in Graphs"*
Honors Thesis Advisor: Tamon C

A. International Research and Scholarly Impact

Summary

My research advances foundational and use-inspired scholarship at the intersection of computing and the science, theory, and applications of **artificial intelligence (AI) that serve as enabling technologies across sectors.** I design core algorithmic frameworks that power discovery in **biotechnology** and the **life sciences**, **healthcare** and **clinical research**, **civil and infrastructure engineering**, **chemistry and materials science**, **cybersecurity and government systems**, the **social sciences and public policy**, and **education and workforce development**. My scholarship has shaped how AI methodologies are deployed not only in molecular and biological discovery but also in **cross-disciplinary knowledge integration, national AI infrastructures, and public-sector innovation**. My publications span premier venues in AI, machine learning, science, engineering, and policy, reflecting a sustained record of high-impact, sector-spanning scholarship.

Selected Indicators of Scholarly Distinction

Robust and sustained scholarly influence. More than **4,500+ citations**, **h-index: 35**, and **102 i10-index** entries, reflecting long-term cross-disciplinary impact in artificial intelligence, computational sciences, engineering, health, biomedicine, chemistry, cybersecurity, policy, and the social sciences.

Extensive and high-impact publication record across sectors. Over **200 refereed publications**, including **79 journal articles**, **74 refereed conference papers**, **42 workshop papers**, and **7 book chapters**, representing sustained productivity across AI, ML, computational biology, engineering analytics, generative chemistry, social computing, cybersecurity, and interdisciplinary science.

Exceptional invited presence and keynote portfolio. Over **100 invited talks** across leading scientific, engineering, health, AI, and policy venues, including keynotes and plenaries at ORNL, SIAM SDM (Blue Sky Award), Salishan, IEEE BIBM, TechConnect, ISMB, NSF institutes, academic research centers, federal agencies, and regional/national innovation forums.

Recognition by premier scientific and professional societies. Elected **Fellow of AIMBE** (2022), **Senior Member of IEEE** (2025), **Member of VASEM** (2024), and recipient of the **SCHEV Outstanding Faculty Award** (2022) and the **Beck Presidential Medal** for Faculty Excellence (2021)—prestigious honors recognizing enduring scholarly excellence and broader scientific impact.

Research excellence recognized through competitive paper awards. Multiple **Best Paper** and **Best Student Paper** Awards and honors across top venues, including the **SIAM SDM Blue Sky Award (2nd place)**, Best Paper and Best Student Paper recognitions at IEEE BIBM, BICoB, and related conferences, highlighting the novelty and influence of my contributions to AI, optimization, and computational sciences.

Significant and sustained competitive research funding. **28 externally funded awards** as PI/co-PI across NSF, AFRL, DoD, SBA, the Commonwealth of Virginia, and industrial partnerships; leadership of multi-year, multi-institutional grants and high-impact awards in AI-enabled discovery, engineering, cybersecurity, digital transformation, and national-scale innovation. Recipient of the **NSF CAREER Award** (2012).

Editorial and scholarly leadership at scale. Over **6 years** as Associate Editor of IEEE/ACM TCBB (2017–2023); Co-Editor and Guest Editor for **10+** interdisciplinary special issues (Robotica, PLoS Computational Biology, Current Opinion in Structural Biology, IJMS); conference leadership roles including General Chair, Program Chair, Senior Program Committee Member, and organizer for AAAI, KDD, ACM BCB, IEEE BIBM, GECCO, ISMB, and more; Reviewer for **top-tier journals** (PNAS, Nature Methods, Nature Communications, Scientific Reports, Bioinformatics, JCI Insight) and major AI/ML/optimization conferences.

National Academies engagement and recognition as a leading AI scholar. Invited contributor and working-group member with the **National Academies of Sciences, Engineering, and Medicine**, including membership on a NASEM Biosecurity Working Group and panelist roles for the Board on Life Sciences on AI, biotechnology, and risk—reflecting recognition as a national leader in AI-enabled science and governance.

Cross-sector scientific reach reflected in publication venues. Research contributions span **8+ major sectors**: biotechnology and life sciences; health and clinical research; chemistry and materials science; engineering systems and infrastructure; cybersecurity and government; social sciences and policy; education and workforce development; and core machine learning / AI theory and algorithmics.

Evidence of field-shaping advances. Pioneered widely adopted methods in **generative and foundation models** for science, **robotics-inspired optimization**, **stochastic search algorithms**, **structural and functional modeling of complex systems**, **interpretable ML**, and **multimodal representation learning**—tooling that underpins discovery pipelines in multiple scientific and economic sectors.

Global research dissemination and translational influence. Research presented to global audiences across **20+** disciplines; algorithms applied in molecular design, chemical generation, structural dynamics, clinical interpretation, infrastructure analytics, cybersecurity, government modernization, public-sector innovation, and national-scale AI policy.

B. Transformational Leadership in Research & Innovation

Summary

My leadership has strengthened Mason's research enterprise and elevated its national profile in AI and interdisciplinary discovery. As the inaugural **Vice President and Chief AI Officer**, former **Associate Vice President for Research** for the Institute for Digital InnovAtion, and current **Associate Dean for Research** (and former **Associate Dean for AI Innovation**) in the College of Engineering and Computing, I have led institution-wide AI strategy, research infrastructure, and public–private partnerships. I architected Mason's **AI² Nexus** strategy across Integrate AI, Inspire AI, Innovate AI, and Impact AI; co-led creation of **PatriotAI**, providing access to more than 1,800 generative AI models; co-led the university taskforce producing the Commonwealth's first use-specific Guidelines for the Responsible Use of AI; founded/co-founded interdisciplinary centers; launched faculty and predoctoral fellowship programs; and built ecosystems that align research, education, workforce development, and external engagement to create durable, scalable models for AI-enabled innovation.

Selected Indicators of Transformational Leadership & Innovation

Inaugural Vice President & Chief AI Officer leading Mason's university-wide AI transformation. Responsible for designing and executing Mason's **AI² Nexus** strategy—the institution's first comprehensive vision for integrating AI across research, education, operations, and public impact. Chair of a **70+ member AI Visioning Taskforce** spanning all academic and non-academic units with student representatives. Led development of Mason's **shared AI vision**, **institutional AI guidelines**, governance structures, and **multi-year implementation roadmaps** for university-wide AI adoption, academic programming, research investment, workforce preparation, and responsible-use policy.

Creation and scaling of AI infrastructure). Architected and led launch of **PatriotAI**, an academic platform that provides students, faculty, and staff with secure access to **1,800+ generative AI models** through use-specific AI agents, integrating governance, literacy, and innovation in partnership with Microsoft and Cloudforce.

Founding and co-founding of major interdisciplinary centers. Founder/Co-founder of high-impact centers that reconfigure Mason's research landscape, including: **Center for AI Innovation & Economic Competitiveness**, **Center of Excellence in Government Cybersecurity Risk Management and Resilience**, **Center for Advancing Human–Machine Partnerships (CAHMP)**, and **Center for Infrastructure Security in the Era of AI**, as well as leadership roles in cross-unit initiatives linking AI, policy, and society.

Strategic leadership within research institutes and P3 ecosystems. As **Associate Vice President for Research** for IDIA, contributed to the early planning and activation of the **Fuse** public–private partnership building at Mason Square by developing criteria and helping identify which labs, faculty, and interdisciplinary teams should relocate to Fuse, shaping its initial research identity and alignment with Mason's strategic priorities.

Transformation of faculty development, research capacity, and team science. Designed and launched innovative faculty and student research capacity programs—including the **IDIA Faculty P3 Fellowships** and the **IDIA Predoctoral Fellowship Program**—that created new pathways for interdisciplinary PhD training, broadened faculty research engagement with industry, and catalyzed large, multi-investigator team science.

College-level research transformation. As **Associate Dean for Research** (and previously for AI Innovation) in the College of Engineering and Computing, driving a data-informed, people-centered strategy to **future-proof the college's research enterprise**: building signature research themes, investing in centers, catalyzing large teams, expanding industry partnerships, and aligning research with regional and national priorities.

Public–private partnerships. Launched the **AI-in-Gov Council** that convenes government CXOs, public-sector technology providers, and Mason faculty and students to co-develop research agendas, pilots, and policy-relevant AI solutions; cultivated strategic relationships with partners including Microsoft and Cloudforce; recognized as a 2025 NVTC **Tech100 Executive Honoree** for advancing innovation ecosystems.

National positioning and institutional visibility for Mason in AI. Represented Mason's AI vision and strategy to the **Board of Visitors** through regular briefings on AI readiness, risk, and opportunity; served as the university's AI lead in high-level engagements with **Micron**, **Accenture Federal**, **NASA Goddard**, **NVTC**, the Council of State Governments, and federal and state agencies. Through invited keynotes, policy panels, and strategy discussions (including National Academies convenings), positioned Mason as a trusted voice in AI innovation, institutional readiness, and responsible-use policy.

National research portfolio leadership. As **NSF Program Director** (CISE/IIS/III), led or co-led **5+ NSF-wide working groups** and cross-directorate initiatives shaping national priorities in AI-enabled discovery and data science. Served as **lead for the NSF COVID-19 RAPID Response** in CISE; **led the HDR: Data Science Corps (DSC)** program, defining a national vision for data science training; and **reoriented the Molecular Foundations for Biotechnology (MFB)** program to make AI a central methodological driver. This leadership was recognized through **two NSF Director's Awards** for COVID-19 coordination and the MFB Working Group.

C. Transformational Leadership in AI Literacy, Education, and Mentorship

Summary

My leadership has reshaped how AI education, literacy, and workforce development are conceived and delivered at George Mason University and across the Commonwealth of Virginia. I have built educational infrastructure that spans a university-wide AI literacy ecosystem (grounded in PatriotAI, LinkedIn Learning curricula, and public-facing AI literacy writing) and statewide AI education frameworks with SCHEV and K–16 partners, preparing students, educators, and institutions for an AI-driven future.

My work integrates curricular design, pedagogical innovation, faculty and staff development, statewide coordination, policy influence, and public–private partnerships, enabling equitable and scalable access to AI literacy across the education continuum. Through this portfolio, I have developed a **national profile as a leading educator and curricula innovator in AI**, regularly advising peer institutions—including **Notre Dame**, **McGill**, **University of Utah**, **CUNY**, **Virginia Tech**, **UVA**, **William and Mary**, and others—on how to build university-wide AI literacy and ecosystems, curricula, governance models, and responsible-use frameworks.

Selected Indicators of Educational Leadership & Innovation

Architect of Mason's university-wide AI literacy ecosystem. Designed and launched the **AI in the Fall → AI in the Spring** ecosystem—integrated training for faculty, staff, and students; tailored workshops; instructional design supports; and curated learning pathways aligned with PatriotAI and LinkedIn Learning–based AI curricula. Delivered high-impact training through events such as the **Innovations in Teaching and Learning Conference** (180+ instructors) and **Faculty & Staff Enrichment Day** (300+ faculty and staff), building campus-wide capacity for responsible AI use.

Creator of statewide AI education frameworks. Appointed to the **SCHEV EO30 AI Taskforce**; co-led the inaugural **Virginia AI in Education Summit**; and authored the **AI in Education Reference Guide**, distributed across the Commonwealth's K–12, community college, and higher education systems—positioning Virginia as a national model for coordinated AI readiness.

Transformational AI curricular innovation. Designed the **AI for All (UNIV 182)** Mason Core course and piloted it with undergraduates, while working with the Provost and Deans to scale the model across all ten colleges. Co-led creation of the **Ethics & AI** undergraduate minor; advise on new certificates, programs, and AI-across-the-curriculum efforts to harmonize initiatives and prepare graduates in all disciplines. Made the AI for All course materials publicly available, further extending Mason's impact.

State-leading graduate AI education. Led design and record-time approval of **Virginia's first Master of Science in Artificial Intelligence**, an interdisciplinary degree addressing statewide and regional workforce needs in emerging AI-intensive fields. The degree is included in the *Advance* module of Virginia's "Virginia Has Jobs in AI" initiative (https://virginiahasjobs.com/ai/).

Professional development at institutional scale. Developed faculty-facing and staff-facing AI pedagogy and workflow programs, reaching hundreds of instructors and staff across colleges. Built institutional structures for responsible AI adoption, classroom integration, course redesign, and student support, embedding AI literacy into teaching and academic support ecosystems.

AI workforce and pipeline development (forward-looking). Leading collaborative efforts with **VDOE**, **VEDP**, **Virginia Works**, **VCCS**, **NOVA**, and K–12 districts to design AI pathways that connect high school, community college, and university experiences; reach pre-service and in-service teachers; and ensure inclusive access to AI competencies across STEM and non-STEM fields.

National visibility and influence. Recognized nationally for AI education leadership by **SCHEV**, **NVTC (Tech100)**, **NSF**, and national AI policy organizations. Invited to write about the AI for All course for **AI Letters**, and maintain a widely-read AI literacy Substack that has expanded Mason's reach to national educator and practitioner communities. Frequently invited to brief policymakers, educators, and institutional leaders on AI literacy, readiness, governance, and implementation, solidifying Mason's and Virginia's roles as leaders in AI education reform.

Deep mentoring footprint and student pipeline. Directed **16 PhD dissertations** and served on numerous additional PhD committees spanning computer science, statistics, bioengineering, systems biology, and related areas. Mentored **40+ undergraduate researchers** and **19 high-school students**, many of whom have co-authored refereed publications, even in first-author capacty, have received competitive awards, and progressed to tenured, tenure-track, and teaching-track faculty, research, and industry leadership roles.

Recognized excellence in teaching and mentorship. Recipient of Mason's **2018 Teaching Excellence Award** and **Outstanding Teaching Award** in Computer Science, as well as the **2013 OSCAR Undergraduate Mentor Excellence Award**, with teaching and mentoring contributions further recognized through the **2022 SCHEV Outstanding Faculty Award**—underscoring the depth and impact of my educational leadership in and beyond the classroom.

D. National-Level Service and Reputation

Summary

My expertise is sought nationally by federal agencies, advisory boards, professional societies, and research consortia. I have played leading roles in shaping national research portfolios, AI and data science education initiatives, AI governance frameworks, and scientific agendas across agencies and sectors. My service portfolio reflects a sustained commitment to guiding national innovation ecosystems and the responsible advancement of computing.

Selected Indicators of National-Level Service & Reputation

National research portfolio leadership at NSF. As **NSF Program Director** (CISE/IIS/III), led or co-led **5+ NSF-wide working groups** and cross-directorate initiatives, influencing national priorities in AI-enabled discovery, data science, and interdisciplinary education. Recognized with **two NSF Director's Awards** for COVID-19 coordination and the MFB Working Group.

National Academies and federal advisory engagements. Served on **National Academies of Sciences, Engineering, and Medicine** working groups in AI, biosecurity, and biotechnology; participated in Board on Life Sciences convenings on AI, biology, and risk; contributed expertise to federal priorities in responsible innovation.

AI risk, governance, and standards leadership. Member of **NIST AI RMF** advisory efforts and working groups on risk management, governance, and generative AI controls; member of the **ACM US Technology Policy Committee**, shaping guidance at the intersection of AI, policy, and digital governance.

Scientific advisory boards and consortia. Service on advisory boards including the **DOE Joint Genome Institute (JGI)**, the **Commonwealth Science & Technology Ethics Policy (STEP) Collaborative**, **NSF Center for Computer-assisted Synthesis (C-CAS)**, and the **UVA ECE** Advisory Board, helping set strategic directions for AI-enabled discovery, ethics, and interdisciplinary science.

Editorial and conference leadership. Associate Editor of **IEEE/ACM TCBB** (6+ years) and Guest/Co-Editor for interdisciplinary special issues in PLoS Computational Biology, IJMS, Robotica, and Current Opinion in Structural Biology; **General Chair** of ACM BCB 2018 and senior program/organizing roles for AAAI, KDD, SDM, ACM BCB, IEEE BIBM, GECCO, and related venues.

Thought leadership and public engagement. Co-founded and co-host the **AI-in-Gov Council** and its podcast series, engaging public-sector leaders on AI governance and implementation. Maintain a national media profile with interviews and features in outlets such as the **Washington Post**, **CIO**, **Fortune**, **WAMU**, **EdTech Magazine**, and more, reinforcing Mason's and Virginia's visibility in AI strategy, policy, and practice.

E. Societal Impact

Summary

My work shapes public policy, strengthens government and public-sector capacity, expands educational opportunity, and accelerates regional and statewide economic development. I have built public–private ecosystems, contributed to state and national AI strategy, developed AI literacy frameworks for K–12 and higher education, and guided organizations on responsible AI adoption. Through research, educational innovation, governance leadership, and community partnerships, I have helped position Virginia—and George Mason University—as models for AI readiness, public-sector modernization, and human-centered innovation.

Selected Indicators of Societal Impact

Statewide leadership in AI education and public readiness. Co-led the **SCHEV EO30 AI Taskforce**, co-hosted the **Virginia AI in Education Summit**, and authored the **AI in Education Reference Guide** distributed across the Commonwealth—advancing AI readiness, literacy, and policy-aligned implementation.

Advancing Virginia's AI strategy and economic development. Collaborated with **VEDP**, **Virginia Works**, **VCCS**, and regional industry partners to align AI workforce pathways, degree programs, and literacy initiatives with high-growth sectors; contributed to "**Virginia Has Jobs in AI**" initiative.

Strengthening government capacity, risk management, and AI governance. Founder of the **AI-in-Gov Council**, a public–private partnership convening government CXOs, federal agencies, and technology leaders on AI governance, risk, and implementation; supported public-sector modernization, cybersecurity resilience, and responsible AI integration through research centers and advisory roles.

Expanding public scientific literacy and civic understanding of AI. Maintain a widely read **AI literacy Substack**, deliver public lectures and workshops, contribute to national media (Washington Post, CIO, Fortune, WAMU, EdTech), and create open resources — extending Mason's reach to educators and broader communities.

Supporting AI access and pathways. Lead collaborations with **K–12 districts**, **NOVA**, **VCCS**, and state partners to expand AI literacy for pre-service and in-service teachers, strengthen dual-enrollment and transfer pipelines, and support upward mobility for underserved and rural learners.

Public-sector innovation through research and interdisciplinary centers. Through centers I have founded, I advance research in national security, biosecurity, workforce development, and digital governance.

F. Appendix

Overview

This appendix provides the evidentiary foundation for the leadership narrative and impact statements presented in Sections A–E. It includes selected publications, grants, advisory roles, invited talks, editorial service, mentoring record, and other professional activities. The subsections below offer quick navigation to each evidence category.

Appendix Contents

F–1. Selected Awards
By the numbers: 30+ competitive distinctions, including AIMBE Fellow, VASEM Member, SCHEV Outstanding Faculty Award, NSF CAREER, and university-level honors.

F–2. External Grants and Funding Portfolio
By the numbers: 29 external awards and 10 internal grants across AI, computational biology, digital transformation, autonomy, defense, security, policy and social sciences, education, and multi-institutional consortia.

F–3. Selected Refereed Publications
By the numbers: 200+ refereed works — 79 journal articles, 74 conference papers, 42 workshop papers, and 7 book chapters.

F–4. Selected Lightly-Refereed Publications
By the numbers: 78 extended abstracts, posters, and short papers presented at major international venues.

F–5. Other Selected Publications and Products
By the numbers: 20+ white papers and technical reports, and 15+ open-source software tools.

F–6. Invited Talks, Keynotes, and Public Engagement
By the numbers: 100+ invited talks and keynotes, 15+ media features (Washington Post, Fortune, WAMU, EdTech, CIO).

F–7. Teaching & Mentoring Record
By the numbers: 16 PhD dissertations, 8 MS theses, 40+ undergraduate researchers, and 19 high-school mentees supervised.

F–8. Professional Service
By the numbers: 10+ editorial roles, 30+ conference/workshop leadership roles, and extensive national reviewing service.

F–9. National and Institutional Leadership
By the numbers: Leadership of 10+ NSF or federal-wide initiatives and major Mason-wide research ecosystem programs.

F1. Awards

Major National & Professional Honors

Tech100 Executive Honoree, Northern Virginia Technology Council, 2025.

IEEE Senior Member, 2025.

Member, Virginia Academy of Science, Engineering, and Medicine (VASEM), 2024.

Fellow, American Institute for Medical and Biological Engineering (AIMBE), 2022.

State Council of Higher Education for Virginia (SCHEV) Outstanding Faculty Award, 2022.

NSF Director's Award (Group), Molecular Foundations for Biotechnology Program Working Group, 2022. *Role: CISE Representative.*

NSF Director's Award (Group), COVID-19 RAPID Coordination Group, 2021. *Role: CISE Coordinator.*

Editor's Choice, Best Paper, and Best Student Paper Awards, 2022, 2019, 2014, 2010.

ACM Service Award for contributions to ACM-BCB, 2013.

NSF CAREER Award, 2012.

Honorable Mention, Humies Competition Award, ACM GECCO, 2012.

University-Level Honors

College of Engineering & Computing Faculty Excellence Award for Research, 2024.

Beck Family Presidential Medal for Faculty Excellence in Research & Scholarship, 2021.

Teaching Excellence Award, 2018.

Emerging Researcher/Scholar/Creator Award, 2014.

OSCAR Undergraduate Mentor Excellence Award, 2013.

Departmental Honors

Outstanding Research Award, Department of Computer Science, 2022.

Outstanding Research Award, Department of Computer Science, 2019.

Outstanding Teaching Award, Department of Computer Science, 2018.

Distinguished Service Award, Department of Statistics, 2017.

Young Faculty Research Award, Department of Computer Science, 2012.

Early Career & Pre-Doctoral Honors

NIH Predoctoral Fellowship, Nanobiology Training Program, 2005–2007.

Clarkson University Presidential Scholarship, 2000–2002; Phi-Mu-Epsilon Fellowship Award for Best Student in Computer Science & Mathematics, 2001; Clarkson University Recognition Day Award, 2001; Hamlin/Darraugh Award; International Student Excellence Award, 2001.

Honorable Mention, International Competition of Mathematics (Turkey), 1997. Winner, National Mathematics Olympiad, Albania, 1994–1998.

F2. Funding

External Funding

29. Hewlett Foundation Gift for "AI for Education Transformation," 09/01/2025 - 08/30/2026.
PI: Warweg P/Schar; Co-PIs: **Shehu A**, Seshaiyer P/COS, Hunter S/CEHD, Lee M/CEC.

28. Commonwealth of Virginia Community Project Award for "George Mason University Center for AI Innovation for Economic Competitiveness," 08/01/2024 - 07/31/2027.
PI: Singh JP/Schar; Co-PIs: **Shehu A**, Clower T/Schar, Kirkpatrick J/CHSS, Koizumi N/Schar.

27. Air Force Research Laboratory: "Digital Transformation Battle Lab," 11/15/2024 - 08/16/2025.
PIs: Josephson B, Archer G. and **Shehu A**.

26. NSF CISE Directorate: Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Conference Grant: "Large Language Models for Biological Discoveries (LLMs4Bio)," 03/01/2024 - 02/28/2025.
PIs: **Shehu A**; co-PIs: Bromberg Y/Emory University, Zhao L/Emory University.

25. Air Force Research Laboratory: "Digital Transformation Battle Lab," 11/15/2023 - 08/16/2024.
PIs: **Shehu A**, Josephson B, Archer G.

24. STTR Air Force: Topic No. AFX23E-TPCSO1-STTR Phase I - Proposal-FX23E-TPCSO1-0061 - "Metadata Overlay for Live-Streaming and Geolocating Security Incident Reporting System," 1/1/2024-3/31/2024.
PIs: Barbara D, **Shehu A**; Industrial partner: Pluribus [AF Contract: FA864924P008].

23. NSF CISE Directorate: Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Medium Collaborative Grant for "Learning Protein-ish: Foundational Insight on Protein Language Models for Better Understanding, Democratized Access, and Discovery," 08/01/2023 - 07/31/2026.
PI: **Shehu A**; co-PI: Bromberg Y/Emory University.

22. NSF BIO Directorate, Infrastructure Innovation for Biological Research (IIBR) Program Grant for "Collaborative Research: IIBR: Innovation: Bioinformatics: Linking Chemical and Biological Space: Deep Learning and Experimentation for Property-Controlled Molecule Generation," 08/01/2023 - 07/31/2026.
PI: **Shehu A**; co-PIs: Wuestl W and Zhang L/Emory University and Minbiole K/Villanova University

21. Commonwealth of Virginia Community Project Award for "Center of Excellence for Furthering U.S. Government Cybersecurity and IT Modernization Leadership and Governance," 09/01/2023 - 08/30/2024.
PI: **Shehu A**; co-PI: Auffret JP, Business/GMU.

20. CIA CHAOTICGOOD DTech Program for "Trustworthy Language Models," 01/01/2023 - 12/31/2023.
PI: Yao Z, CS/GMU; co-PIs: **Shehu A**; Liu M, CS/GMU.

19. U.S. Department of Defense MINERVA Research Initiative Award for "The Cultural, Economic, and Institutional Determinants of AI Infrastructures and their Consequences in Global Contexts," 07/01/2022 - 06/30/2025.   PI: Singh JP/GMU; co-PI: **Shehu A**; SP: Anastasopolous A/GMU; Kirkpatrick J/GMU; Hunzinger M/GMU.

18. Commonwealth of Virginia, Alzheimer's and Related Diseases Research Award for "Mechanisms of Amyloid Interaction and Signaling through the Nicotinic Receptor," 08/01/2019 - 06/39/2022.
PI: Kabbani N/GMU; co-PIs: **Shehu A**; Lucchini A/GMU.

17. NSF Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Small Grant for "Graph Generative Deep Learning for Protein Structure Prediction," 07/18/2018 - 07/31/2022.
PI: **Shehu A**; co-PI: Zhang L/GMU.

16. NSF Foundations of Emerging Technologies (FET): Collaborative Medium Grant for "Automated Analysis and Exploration of High-dimensional and Multimodal Molecular Energy Landscapes," 07/26/2019 - 07/31/2023.   PIs: **Shehu A** and Plaku E/CUA; co-PI: Qiao W/GMU.

15. Jeffress Trust Awards Program in Interdisciplinary Research Award for "Modeling Protein Structure via Graph Generative Deep Learning," 06/30/2019 - 05/31/2020.   PI: Zhang L/IST-GMU; co-PI: **Shehu A**.

14. NSF Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Collaborative Medium Grant for "Guiding Exploration of Protein Structure Spaces with Deep Learning," 07/01/2018 - 06/30/2021.   PIs: **Shehu A** and Chen J/UMissouri.

13. NSF Division of Mathematics Sciences (DMS) Grant for "Statistical Inference for Molecular Landscapes," 08/01/2018 - 07/31/2021.   PI: Qiao W/Statistics-GMU; co-PI: **Shehu A**.

12. Jeffress Trust Awards Program in Interdisciplinary Research Award for "High-dimensional Statistics and Biomolecular Modeling as a Powerful Microscope over Pathogenic Mutations in Proteinopathies," 06/15/2017 - 06/14/2018.   PI: Qiao W/Statistics-GMU; co-PI: **Shehu A**.

11. REU Supplement for NSF CCF Grant For "Novel Stochastic Optimization Algorithms for Advancing the Treatment of Dynamic Molecular Systems," 02/01/2017 - 06/30/2018.   PI: **Shehu A**; co-PI: De Jong, K.

10. REU Supplements for NSF CAREER Grant for "Probabilistic Methods for Addressing Complexity and Constraints in Protein Systems," 09/01/2016-02/01/2018.   PI: **Shehu A**, no co-PIs.

9. PFP/DARPA to PI: Stavrou A for "Enhanced Cyber Defense by Leveraging Involuntary Analog Emissions", Summer 2016.   Faculty Associate: **Shehu A**.

8. NSF Software Infrastructure for Sustained Innovation (Sustainable Software Elements – SSE) Collaborative Grant for "A Novel Plug-and-play Software Platform of Robotics-inspired Algorithms for Modeling Biomolecular Structures and Motions," 02/01/2015 - 01/31/2018.   PIs: **Shehu A**, Plaku E/CUA, Roitberg A/UF.

7. NSF Computing Core Foundations (CCF): Algorithmic Foundations (AF) Grant for "Novel Stochastic Optimization Algorithms for Advancing the Treatment of Dynamic Molecular Systems," 07/1/2014 - 06/30/2018.   PI: **Shehu A**; co-PI: De Jong, K.

6. NSF CISE Grant for "NSF CISE CAREER Writing Workshop," 12/05/2013 - 05/31/2014.   PI: **Shehu A**; co-PI: Rangwala H/Computer Science-GMU.

5. Jeffress Trust Awards Program in Interdisciplinary Research Award for "Probabilistic Search Algorithms: Powerful Novel Tools for Peptide Modeling," 09/15/2013 - 06/15/2015.
            PI: **Shehu A**; co-PI: Blaisten-Barojas E/Computational Materials Science-GMU.

4. NSF REU Supplement for NSF CAREER Grant for "Probabilistic Methods for Addressing Complexity and Constraints in Protein Systems," 07/01/2013-06/30/2014.   PI: **Shehu A**, no co-PIs.

3. Virginia Foundation for Healthy Youth Award for "Molecular Mechanisms Underlying Menthol Cigarette Addiction," 07/01/2013 - 10/31/2015.   PI: Kabbani N/Neuroscience-GMU; co-PI: **Shehu A**.

2. NSF Information and Intelligent Systems (IIS): Robust Intelligence (RI) CAREER Grant for "Probabilistic Methods for Addressing Complexity and Constraints in Protein Systems," 03/01/2012 - 02/28/2017.
                PI: **Shehu A**, no co-PIs.

1. NSF Computing Core Foundations (CCF): Algorithmic Foundations (AF) Grant for "A Unified Computational Framework to Enhance the Ab-initio Sampling of Native-like Protein Conformations," 9/1/2010 - 8/31/2014.   PI: **Shehu A**, no co-PIs.

Internal Funding

10. Curriculum Impact Grant for "Ethics and AI," Cross-Disciplinary Undergraduate Minor 06/01/2020-05-31/2022.   PIs: **Shehu A**/CS-GMU, Jones R/PHI-GMU, Kirkpatrick J/PHI-GMU, Monea A/Cultural Studies-GMU, and Warweg P/CAHMP.

9. Provost's Transdisciplinary Center for Advanced Study Award for the "Center for Advancing Human-Machine Partnerships (CAHMP)," 08/25/2019-07-30/2024. PIs: **Shehu A**/CS-GMU, Lattanzi D/CEIE-GMU, and Bannan B/CEHD-GMU.

8. GMU Multidisciplinary Seed Funding Initiative in Modeling, Simulation, and Data Analytics for "An Integrative Multi-disciplinary Approach to Unravel and Target Viral Replication," 09/07/2017-05/31/2019).
PI: **Kehn-Hall K/SSB-GMU**, co-PIs: **Shehu A**/CS-GMU and Blaisten-Barojas E/CDS-GMU.

7. Mason Seed Grant for "Towards A Unified Dry to Wet Laboratory Framework for Screening, Modifying, and Designing Antimicrobial Peptides," 12/20/2013-05/01/2014.
PI: **Shehu A**, co-PI: Vidyashankar A/Statistics-GMU.

6. Mason Seed Grant for "Structural and Functional Mechanisms Underlying Menthol Addiction," 07/01/2013-10/01/2013.   PI: Kabbani N/Neuroscience-GMU, co-PI: **Shehu A**.

5. Mason Seed Grant for "Probabilistic Search Techniques as New Tools for Peptides Modeling," 12/01/2012-06/01/2013.   PI: **Shehu A**, co-PI: Cortes J/Robotics-University of Toulouse, France.

4. Mason Seed Grant for "Combining Experiment and Computation to Characterize Dopamine Receptors and the Mode of Action of Antipsychotic Drugs," 06/01/2010-06/01/2011.
                PI: Kabbani N/Neuroscience-GMU, co-PI: **Shehu A**.

3. RA Support to Shehu, AY 2010-2011.

2. Bioengineering Seed Grant for "Staying Ahead of Evolution: Engineering Novel Antimicrobial Peptides," 01/01/2009-12/31/2010.   PI: **Shehu A**, co-PIs: Bishop B/Biochemistry-GMU and van Hoek M/Molecular Biology-GMU.

1. Mason Seed Grant for "In-silico Characterization and Design of Protein Complexes: Exploiting Symmetry and Redundancy," 01/01/2009-12/31/2009.   PI: **Shehu A**.

F3. Refereed Publications

Summary

Articles are listed in reverse chronological order. Shehu's advisees are indicated by (p) for postdoctoral, (g) for graduate, (u) for undergraduate, and (h) for high-school students. Corresponding authors are indicated by (*). Impact factors (IF) reported for journal publications are those at the year of publication. If not available, 5-year average or most recent values are reported. Acceptance Rates (AR) are reported for conference and workshop papers where available, whether obtained online or as reported in published proceedings.

Refereed Journal Publications

J79 Tang M, Cromie GA, Kabir A^g, Timour MS, Ashmead J, Lo RS, DiMaio F, Morizono H, Caldovic L, Mew NA, Gropman A, **Shehu A*** and Dudley AM*. *Predicting Epistasis Across Proteins by Structural Logic. Proc Natl Acad USA*, 2026 (out of embargo, going live on Jan 12, 2026).   [IF: 9.1]

J78 **Shehu A***. *Beyond the Singularity Myth: Artificial General Intelligence as Cumulative Infrastructural Transformation - Absorption Capacity, Epistemic Drift, and the Erosion of Human Verification Power. ACM Transactions on Intelligent Systems and Technology (TIST)*, 2025 (invited vision article). DOI: 10.1145/3779133. [IF: 6.6]

J77. Dua M^g, Singh JP*, and **Shehu A***. *The Ethics of National Artificial Intelligence Plans: An Empirical Lens. The AI and Ethics Journal* 5(1), Springer 2025.   [IF: 3.5]

J76. Singh JP*, **Shehu A**, Wesson C^g, and Dua M^g. *Entangled Narratives: Insights from Social and Computer Sciences on National Artificial Intelligence Infrastructures. International Studies Quarterly* 69(1): sqaf001, 2025.   [IF: 2.4]

J75. Kabir A^{g,*}, Bhattarai M, Rasmussen K, **Shehu A**, Bishop A, Alexandrov B S, and Usheva A. *DNA Breathing Dynamics and Deep Learning for Predicting Human Genome-wide Transcription Factor Binding Sites. Nucleic Acids Research* gkae783, 2024.   [IF: 16.6]

J74. Kabir A^g, Moldwin A^g, Bromberg Y, and **Shehu A***. *In the Twilight Zone of Protein Sequence Homology: Do Protein Language Models Learn Protein Structure?. Bioinformatics Advances* vbae119, 2024.   [IF: 2.4]

J73. Lian Y^g, Bodian D, and **Shehu A***. *Elucidating the Role of Wildtype and Variant FGFR2 Structural Dynamics. Intl J Mol Sci* 25(8): 4523, 2024.   [IF: 5.6]

J72. Bromberg Y*, Kabir A^g, Ramakrishnan P, and **Shehu A***. *Variant Prediction in the Age of Machine Learning. Machine Learning and Protein Science*, Cold Spring Harb Perspect Biol a041467, 2023. [IF: 1.92]

J71. Kabir A^{g,*}, Bhattarai M*, Rasmussen K, **Shehu A**, Usheva A, Bishop AR, and Alexandrov BS. *Dynamically Active Zone of DNA Breathing. Bioinformatics* 39(11):btad699, 2023.   [IF: 5.8]

J70. Kabir A^g and **Shehu A***. *GOProFormer: A Multi-Modal Transformer Method for Gene Ontology Protein Function Prediction. Biomolecules* 12(11):1709, 2022.   [IF: 6.604]

J69. Qiao W* and **Shehu A**. *Space Partitioning and Regression Mode Seeking via a Mean-Shift-Inspired Algorithm. Electronic Journal of Statistics* 16(2):5623-5658, 2022.   [IF: 1.125]

J68. Kabir KL^g, Ma B, Nussinov R, and **Shehu A***. *Fewer Dimensions, More Structures for Improved Discrete Models of Dynamics of Free versus Antigen-Bound Antibody. Biomolecules* 12(7):1011, 2022.   [IF: 6.604]

J67. Alam FF^g and **Shehu A***. *Data Size and Quality Matter: Generating Physically-realistic Distance Maps of Protein Tertiary Structures. Biomolecules* 12(7):908, 2022 (featured on issue cover),
<u>*Editor's Choice 2022 Award.*</u>   [IF: 6.604]

J66. Du Y^u, Guo X^g, **Shehu A**, and Zhao, L*. *Controlling the Generation of Molecules via Interpretable Variational Autoencoders. Bioinformatics* , btac296, 2022.   [IF: 5.610]

J65. Kamranfar P^g, Lattanzi D Y*, **Shehu A***, and Stoffels S. *Pavement Distress Recognition via Wavelet-based Clustering of Smartphone Accelerometer Data. ASCE J of Computing in Civil Engineering*, 2021 (in press). [IF: 5.44]

J64. Guo X^g, Du Y^u, Tadepalli S^g, Zhao L, and Amarda Shehu**Shehu A***. *Generating Tertiary Protein Structures via Interpretable Graph Variational Autoencoders. Bioinformatics Advances* 1:1(vbab036), 2021. [IF: 2.833]

J63. Zaman AB^g, Inan TT^g, De Jong KA, and **Shehu A***. *Adaptive Stochastic Optimization to Improve Protein Conformation Sampling. IEEE/ACM Trans Comput Biol and Bioinf (TCBB)*, 2021, online ahead of print (DOI: 10.1109/TCBB.2021.3134103).   [IF: 3.015]

J62. Gogovi G^g, Silayi S^g, and **Shehu A***. *Computing the Structural Dynamics of RVFV L Protein Domain in Aqueous Glycerol Solutions. Biomolecules* 11(10):1427, 2021.   [IF: 4.8797]

J61. Rahman T^g, Du Y^u, Zhao L, and **Shehu A***. *Generative Adversarial Learning of Protein Tertiary Structures. Molecules* 26(5):1209, 2021.   [IF: 3.267]

J60. Akhter N^g, Kabir KL^g, Chennupati G, Vangara R, Alexandrov BS, Djidjev H, and **Shehu A***. *Improved Protein Decoy Selection via Non-Negative Matrix Factorization. IEEE/ACM Trans Comput Biol and Bioinf (TCBB)*, 2021, online ahead of print (DOI: 10.1109/TCBB.2020.3049088). [IF: 3.015]

J59. Alam FF^g and **Shehu A***. *Unsupervised Multi-Instance Learning for Protein Structure Determination. J Bioinf and Comput Biol (JBCB)* 19(1):2140002, 2021. [IF: 1.063]

J58. Hoseini P^p, Zhao L, and **Shehu A***. *Generative Deep Learning for Macromolecular Structure and Dynamics. Curr Opin in Struct Biol*, Section on Theory and Simulation/Computational Methods 67: 170-177, 2021 (invited). [IF: 7.108]

J57. Bin Zaman A^g, Kamranfar P^g, Domeniconi C, and **Shehu A***. *Reducing Ensembles of Protein Tertiary Structures Generated De Novo via Clustering. Molecules* 25(9), 2228, 2020. [IF: 3.998]

J56. Tadepalli S^g, Barbara D, and **Shehu A***. *Anomaly Detection-based Recognition of Near-Native Protein Structures. IEEE Transactions on NanoBioscience* 19(3): 562-570, 2020. [IF: 1.955]

J55. Akhter N^g, Chennupati G, Djidjev H, and **Shehu A***. *Decoy Selection for Protein Structure Prediction Via Extreme Gradient Boosting and Ranking. BMC Bioinf* 21(Suppl 1):189,2020. [IF: 2.213]

J54. Alam FF^g, Rahman T^g, and **Shehu A***. *Evaluating Autoencoder-based Featurization and Supervised Learning for Protein Decoy Selection. Molecules* 25(5), 1146, 2020. [IF: 3.998]

J53. McDermott-Roe C*, Lu W, Maximova T^p, Wada S, Bukowy J, Marquez M, Lai S, **Shehu A**, Benjamin I, Geurts A, and Musunuru, K. *Investigation of a dilated cardiomyopathy–associated variant in BAG3 using genome-edited iPSC-derived cardiomyocytes. J of Clinical Investigation (JCI) Insight*, 4(22):e128799, 2019. [IF: 6.014]

J52. Kabir KL^g, Akhter N^g, and **Shehu A***. *From Molecular Energy Landscapes to Equilibrium Dynamics via Landscape Analysis and Markov State Models. J Bioinf and Comp Biol* 17(6):1940014, 2019. [IF: 0.845]

J51. Akhter N^g, Chennupati G, Kabir KL^g, Djidjev H, and **Shehu A***. *Unsupervised and Supervised Learning over the Energy Landscape for Protein Decoy Selection. Biomolecules,* 9(1): 607, 2019. [IF: 4.694]

J50. Zaman ABB^g and **Shehu A***. *Building Maps of Protein Structure Spaces in Template-free Protein Structure Prediction. J Bioinf and Comp Biol* 17(6):1940013, 2019. [IF: 0.845]

J49. Zaman AB^g and **Shehu A***. *Balancing Multiple Objectives in Conformation Sampling to Control Decoy Diversity in Template-free Protein Structure Prediction. BMC Bioinf* 20, 211, 2019. [IF: 2.511]

J48. Gogovi G^g, Almsned F^g, Ricci N^g, Kehn-Hall K, **Shehu A**, and Blaisten-Barojas E*. *Modeling the Tertiary Structure of the Rift Valley Fever Virus L protein. Molecules* 24(3), 781, 2019. [IF: 3.060]

J47. Kabir KL^g, Hassan L^g, Rajabi^g, and **Shehu A***. *Graph-based Community Detection for Decoy Selection in Template-free Protein Structure Prediction. Molecules* 24(3), 741, 2019. [IF: 3.060]

J46. Nussinov R, Tsai C-J, **Shehu A**, and Jang, H. *Computational Structural Biology: The Challenges Ahead. Molecules* 24(3), 673, 2019. [IF: 3.060]

J45. Morris D^g, Maximova T^p, Plaku E, and **Shehu A***. *Attenuating Dependence on Structural Data in Computing Protein Energy Landscapes. BMC Bioinf* 20 (Suppl11), 280, 2019. [IF: 2.511]

J44. Qiao W, Akhter N^g, Fang X^u, Maximova T^p, and **Shehu A***. *From Mutations to Mechanisms and Dysfunction via Computation and Mining of Protein Energy Landscapes. BMC Genom* 19 (Suppl 7): 671, 2018. [IF: 3.501]

J43. Akhter N^g, Qiao W, and **Shehu A***. *An Energy Landscape Treatment of Decoy Selection in Template-free Protein Structure Prediction. Computation* 6(2):39, 2018 (invited to special issue on "Computation in Molecular Modeling"). [IF: 1.821]

J42. Veltri D, Kamath U, and **Shehu A***. *Deep Learning Improves Antimicrobial Peptide Recognition. Bioinformatics* 34(16), 2740-2747, 2018. [IF: 4.531]

J41. Akhter N^g and **Shehu A***. *From Extraction of Local Structures of Protein Energy Landscapes to Improved Decoy Selection in Template-free Protein Structure Prediction. Molecules* 23(1): 216, 2018. [IF: 3.060]

J40. Maximova T^p, Zhang Z, Carr DB, Plaku E, and **Shehu A***. *Sample-based Models of Protein Energy Landscapes and Slow Structural Rearrangements. J Comput Biol* 25(1):33-50, 2017. [IF: 1.191]

J39. Sapin E^p, De Jong K*, and **Shehu A***. *From Optimization to Mapping: An Evolutionary Algorithm for Protein Energy Landscapes. IEEE/ACM Trans Comput Biol and Bioinf* 15(3):719-731, 2018. [IF: 2.896]

J38. Maximova T^p, Plaku E*, and **Shehu A***. *Structure-guided Protein Transition Modeling with a Probabilistic Roadmap Algorithm. IEEE/ACM Trans Comput Bio and Bioinf*, 2017. [IF: 2.428]

J37. Veltri D^g, Kamath U, and **Shehu A***. *Improving Recognition of Antimicrobial Peptides and Target Selectivity through Machine Learning and Genetic Programming. IEEE/ACM Trans Comput Biol and Bioinf* 14(2):1545-5963, 2017. [IF: 2.428]

J36. **Shehu A**[*] and Plaku E[*]. *A Survey of Computational Treatments of Biomolecules by Robotics-inspired Methods Modeling Equilibrium Structure and Dynamics. J Artif Intel Res* 597: 509-572, 2016.   [IF: 2.284]

J35. Sapin E[p], Carr DB, De Jong K[*], and **Shehu A**[*]. *Computing energy landscape maps and structural excursions of proteins. BMC Genom* 17(Suppl 4): 546, 2016.   [IF: 3.12]

J34. Molloy K[g], Clausen R[g], and **Shehu A**[*]. *A Stochastic Roadmap Method to Model Protein Structural Transitions. Robotica* 34(8): 1705-1733 *(featured on issue cover)*, 2016.   [IF: 0.89]

J33. Molloy K[g] and **Shehu A**[*]. *A General, Adaptive, Roadmap-based Algorithm for Protein Motion Computation. IEEE Trans NanoBioScience* 15(2): 158-165, 2016.   [IF: 1.77]

J32. Maximova T[p], Moffat R[g], Ma B, Nussinov R, and **Shehu A**[*]. *Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Comput Biol* 12(4): e1004619, 2016, *(top 50 most downloaded for 2016 and featured on issue cover and PLoS Comput Biol blog).*   [IF: 4.83]

J31. **Shehu A**[*] and Nussinov R[*]. *Computational Methods for Exploration and Analysis of Macromolecular Structure and Dynamics. PLoS Comput Biol* 11(10): e1004585, 2015 *(editorial).*   [IF: 4.83]

J30. Devaurs D, Molloy K[g], Vaisset M, **Shehu A**, Simeon T, and Cortes J[*]. *Characterizing Energy Landscapes of Peptides using a Combination of Stochastic Algorithms. IEEE Trans NanoBioScience* 14(5): 545-552, 2015.   [IF: 1.77]

J29. Hashmi I[g] and **Shehu A**[*]. *idDock+:Integrating Machine Learning in Probabilistic Search for Protein-protein Docking. J Comput Biol* 22(9): 806-822, 2015.   [IF: 1.67]

J28. Clausen R[g] and **Shehu A**[*]. *A Data-driven Evolutionary Algorithm for Mapping Multi-basin Protein Energy Landscape. J Comput Biol* 22(9): 844-860, 2015.   [IF: 1.67]

J27. Clausen R[g], Ma B, Nussinov R[*], and **Shehu A**[*]. *Mapping the Conformation Space of Wildtype and Mutant Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. PLoS Comput Biol* 11(9): e1004470, 2015.   [IF: 4.83]

J26. Kamath U[g], De Jong KA[*], and **Shehu A**[*]. *Effective Automated Feature Construction and Selection for Classification of Biological Sequences. PLoS One* 9(7): e99982, 2014.   [IF: 5.2]

J25. Molloy K[g], Van JM[u], Barbara D, and **Shehu A**[*]. *Exploring Representations of Protein Structure for Automated Remote Homology Detection and Mapping of Protein Structure Space. BMC Bioinf*, 15(Suppl 8): S4, 2014.   [IF: 3.02]

J24. Kabbani, N[*], Nordman JC, Corgiat B, Veltri D[g], **Shehu A**, and Adams DJ. *Are Nicotinic Receptors Coupled to G Proteins? Bioessays*, 35(12):1025-1034, 2013 *(video abstract).*   [IF: 5.42]

J23. Ashoor A, Nordman JC, Veltri D[g], Yang KS, Al Kury L, Shuba Y, Mahgoub M, Howarth FC, Lupica C, **Shehu A**, Kabbani N, and Oz M[*]. *Menthol Inhibits 5-HT3 Receptor-mediated Currents. J of Pharmacology and Experimental Therapeutics* 347(20:398-409, 2013 *(issue front cover).*   [IF: 4.31]

J22. Ashoor A, Nordman JC, Veltri D[g], Yang KS, Al Kury L, Shuba Y, Mahgoub M, Howarth FC, Sadek B, **Shehu A**, Kabbani N, and Oz M[*]. *Menthol Binding and Inhibition of Alpha7-nicotinic Acetylcholine Receptors. PLoS One* (8)7:e67674, 2013 *(top 25% most cited as of June 2017).*   [IF: 4.09]

J21. Molloy M[g], Saleh S[u], and **Shehu A**[*]. *Probabilistic Search and Energy Guidance for Biased Decoy Sampling in Ab-initio Protein Structure Prediction. IEEE/ACM Trans Comput Biol and Bioinf*, 10(5):1162-1175, 2013.   [IF: 2.25]

J20. Hashmi I[g] and **Shehu A**[*]. *HopDock: A Probabilistic Search Algorithm for Decoy Sampling in Protein-protein Docking. Proteome Sci* 11(Suppl 1):S6, 2013.   [IF: 2.42]

J19. Saleh S[u], Olson B[g], and **Shehu A**[*]. *A population-based Evolutionary Search Approach to the Multiple Minima Problem in de novo Protein Structure Prediction. BMC Struct Biol* 13(Suppl 1): S4, 2013.   [IF: 2.10]

J18. Olson B[g] and **Shehu A**[*]. *Rapid Sampling of Local Minima in Protein Energy Surface and Effective Reduction through a Multi-objective Filter.* Proteome Sci 11(Suppl 1):S12, 2013.   [IF: 2.42]

J17. Molloy M[g] and **Shehu, A**[*]. *Elucidating the Ensemble of Functionally-relevant Transitions in Protein Systems with a Robotics-inspired Method. BMC Struct Biol* 13(Suppl 1):S8, 2013.   [IF: 2.09]

J16. Olson B[g], Hashmi I[g], Molloy K[g] and **Shehu, A**[*]. *Basin Hopping as a General and Versatile Optimization Framework for the Characterization of Biological Macromolecules. Advances in Artificial Intelligence J*, 674832, 2012 (special issue1 on applications in biomedicine).

J15. Olson B[g] and **Shehu A**[*]. *Evolutionary-inspired Probabilistic Search for Enhancing Sampling of Local Minima in the Protein Energy Surface. Proteome Sci*, 10(Suppl1): S5, 2012.   [IF: 2.42]

J14. Hashmi I[g], Akbal B, Haspel N, and **Shehu A**[*]. *Guiding Protein Docking with Geometric and Evolutionary*

Information. J Bioinf and Comp Biol, 10(3): 1242008, 2012.   [IF: 1.06]

J13. Akbal B, Hashmi I^g, **Shehu A**, and Haspel N*. *An Evolutionary Conservation Based Method for Refining and Reranking Protein Complex Structures. J Bioinf and Comp Biol*, 10(3): 12420024, 2012.   [IF: 1.06]

J12. Olson B^g, Molloy^g, K, Hendi S-F^g, and **Shehu A***. *Guiding Probabilistic Search of the Protein Conformational Space with Structural Profiles. J Bioinf and Comp Biol*, 10(3): 1242005, 2012.   [IF: 1.06]

J11. **Shehu A*** and Kavraki LE*. *Modeling Structures and Motions of Loops in Protein Molecules. Entropy J*, 14(2):252-290, 2012 (invited review article).   [IF: 1.11]

J10. Kamath U^g, Compton J^u, Islamaj-Dogan R, De Jong KA*, and **Shehu A***. *An Evolutionary Algorithm Approach for Feature Generation from Sequence Data and its Application to DNA Splice-Site Prediction. IEEE Trans Comput Biol and Bioinf*, 9(5):1387-1398, 2012.   [IF: 2.25]

J9. Kamath U^g, **Shehu A***, and De Jong KA*. *A Two-Stage Evolutionary Approach for Effective Classification of Hypersensitive DNA Sequences. J Bioinf and Comp Biol*, 9(3):399-413, 2011.   [IF: 1.06]

J8. Olson B^g, Molloy K^g and **Shehu A***. *In Search of the Protein Native State with a Probabilistic Sampling Approach. J Bioinf and Comp Biol*, 9(3):383-398, 2011.   [IF: 1.06]

J7. **Shehu A*** and Olson B^g. *Guiding the Search for Native-like Protein Conformations with an Ab-initio Tree-based Exploration. Intl J of Robot Res*, 29(8):1106-1127, 2010.   [IF: 4.93]

J6. Hegler JA, Laetzer J, **Shehu A**, Clementi C, and Wolynes, PG*. *Restriction vs. Guidance: Fragment Assembly and Associative Memory Hamiltonians for Protein Structure Prediction. Proc Natl Acad Sci USA*, 106(36):15302-15307, 2009.   [IF: 9.54]

J5. **Shehu A**, Clementi C*, and Kavraki LE*. *Multiscale Characterization of Protein Conformational Ensembles. Proteins: Struct Funct Bioinf*, 76(4):837-851, 2009.   [IF: 3.03]

J4. **Shehu A**, Kavraki LE, and Clementi C*. *Unfolding the Fold of Cyclic Cysteine-rich Peptides. Protein Sci* 17(3):482-493, 2008.   [IF: 3.11]

J3. **Shehu A**, Clementi C, and Kavraki LE*. *Sampling Conformation Space to Model Equilibrium Fluctuations in Proteins. Algorithmica* 48(4):303-327, 2007.   [IF: 0.89]

J2. **Shehu A**, Kavraki LE, and Clementi C*. *On the Characterization of Protein Native State Ensembles. Biophys J* 92(5):1503-1511, 2007.   [IF: 4.53]

J1. **Shehu A**, Clementi C*, and Kavraki LE*. *Modeling Protein Conformational Ensembles: From Missing Loops to Equilibrium Fluctuations. Proteins: Struct Funct Bioinf* 65(1):164-179, 2006.   [IF: 3.88]

Refereed Conference Publications

C74. Pan B, Ghaemi S^g, Consylman AJ, Zhao Z, Petersen AA, Wu A, Chang G, McDonough D, Forman MA, Bezold EL, Wuest WM, Minbiole K, Zhao L, and **Shehu A***. *Generating Quaternary Ammonium Compound Structures via an Instructible Chemist-AI Alignment Framework.* In Proc ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), Toronto, CA, 2025.

C73. Inan TT^g, Shultana S^g, and **Shehu A***. *Closing the Gap between Optimization and Generation in Deep Learning with A Multi-Objective Evolutionary Algorithm.* In Proc Genet and Evol Comp Conf (ACM GECCO), Málaga, Spain, 2025.

C72. Bromberg Y* and **Shehu A***. *Blue Sky Paper: Better AI For Understanding Life on Earth: Predict First, Design Later.* SIAM International Conference on Data Mining (SDM), Alexandria, VA 2025.
     Second Place Winner of the Blue Sky Best Research Paper Awards at SIAM SDM 2025..

C71. Blouir S^g, Smith J, Anastasopoulos A, and **Shehu A***. *Birdie: Advancing State Space Models with a Minimalist Architecture and Novel Pre-training Objectives.* 2024 Conference on Empirical Methods in Natural Language Processing (EMNLP), Miami, FL 2024.

C70. Singh JP*, Dua M^g, and **Shehu A***. *Diffusion of Power and Multiplexed Governance: Evolving Networks and Clusters for Global Governance of Artificial Intelligence Infrastructures.* 17th Conference on the Political Economy of International Organization (PEIO), Harvard University, MA 2025, pg. 1-35.

C69. Dua M^g, Singh JP, and **Shehu A***. *Health Equity in AI Development and Policy: An AI-enabled Study of International, National and Intra-national AI Infrastructures.* AAAI Fa24 Machine Intelligence for Equitable Global Health (MI4EGH) Symposium, Fall Symposium Series, Arlington, VA 2024, pg. 1-8.

C68. Inan TT^g and **Shehu A***. *Revisiting Evolutionary Algorithms for Optimization for Deep Learning: Introducing DL-HEA.* In Proc Genet and Evol Comp Conf (ACM GECCO), Melbourne, Australia 2024.

C67. Bao Y, **Shehu A**, and Liu M*. *Global Convergence Analysis of Local SGD for One-hidden-layer Convolutional Neural Network without Overparameterization.* Thirty-seventh Conference on Neural Information Processing

Systems (NeurIPS), New Orleans, Louisiana, 2023.

C66. Singh JP*, **Shehu A***, Wesson C[g], and Dua M[g]. *The Cultural, Economic, and Institutional Determinants in National Artificial Intelligence Infrastructures: Insights from Social and Computer Sciences.* International Studies Association (ISA), Montreal, CA, 2023.

C65. Hunziker MA, Dua M[g], and **Shehu A***. *What can Artificial Intelligence Tell Us About American Grand Strategy?* International Studies Association (ISA), Montreal, CA, 2023.

C64. Wang S[g], Guo X[g], Lin M[g], Pan B[g], Du Y[g], Wang Y[u], Ye Y[u], Petersen AA[g], Leitgeb A[g], Alkhalifa S, Minbiole K, Wuest W, **Shehu A**, and Zhao L*. *Multi-objective Deep Data Generation with Correlated Property Control.* Conf on Neural Information Processing Systems (NeurIPS), New Orleans, LA, 2022.
[AR: 25.6%]

C63. Kabir A[g] and **Shehu A***. *Sequence-Structure Embeddings via Protein Language Models Improve on Prediction Tasks.* IEEE Intl Conf on Knowledge Graphs (ICKG), Orlando, FL, 2022.

C62. Inan T[g], Liu M, and **Shehu A***. *F-Measure Optimization for Multi-Class, Imbalanced Emotion Classification Tasks.* Intl Conf on Artificial Neural Networks (ICANN), Bristol, UK, 2022.

C61. Du Y[u], Guo X, **Shehu A**, and Zhao L*. *Interpretable Molecular Graph Generation via Monotonic Constraints.* In Proc SIAM International Conference on Data Mining (SDM), Alexandria, VA, 2022, pg. 1-9.
[AR: 28%]

C60. Zaman AB[g], De Jong KA, and **Shehu A***. *Guiding Protein Conformation Sampling with Conformation Space Maps.* In Proc Intl Conf on Bioinf and Comput Biol (BICOB), Virtual, 2022, pg. 1-11, *Finalist for Best Paper Award.*.

C59. Kabir A[g], Inan TT[g], and **Shehu A***. *Analysis of AlphaFold2 for Modeling Structures of Wildtype and Variant Protein Sequences.* In Proc Intl Conf on Bioinf and Comput Biol (BICOB), Virtual, 2022, pg. 1-12 *Best Paper Award.*

C58. Kabir KL[g], Bhattarai M, Alexandrov BS, and **Shehu A***. *Single Model Quality Estimation of Protein Structures via Non-negative Tensor Factorization.* In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), Virtual, 2021, pg. 1-10.

C57. Rahman T[g], Du Y[u], and **Shehu A***. Graph Representation Learning for Protein Conformation Sampling. In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), Virtual Virtual, 2021, pg. 1-10.

C56. Vajre V[h], Naylor M, Kamath U, and **Shehu A***. PsychBERT: A Mental Health Language Model for Social Media Mental Health Behavioral Analysis. In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Virtual, 2021, pg. 1-8.
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C55. Du Y[u], Wang Y[u], Alam FF[g], Lu Y[u], Guo X[g], Liang Zhao, and **Shehu A***. *Deep Latent-Variable Models for Controllable Molecule Generation.* In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Virtual, 2021, pg. 1-6.
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C54. Rajabi Z[g], Uzuner O, and **Shehu A***. *Detecting Scarce Emotions Via BERT and Hyperparameter Optimization.* In Proc Intl Conf on Artificial Neural Networks (ICANN), Virtual, 2021, pg. 1-12.

C53. Kabir KL[g], Chennupati G, Vangara R, Djidjev H, Alexandrov B, and **Shehu A***. *Decoy Selection in Protein Structure Determination via Symmetric Non-negative Matrix Factorization.* In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), 2020, pg. 23-28.
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C52. Zaman AB[g], Inan TT[g], and **Shehu A***. *Protein Decoy Generation via Adaptive Stochastic Optimization for Protein Structure Determination.* In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), 2020, pg. 50-55.
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C51. Alam FF[g] and **Shehu A***. *Variational Autoencoders for Protein Structure Prediction.* In Proc ACM Conf on Bioinf and Comp Biol (BCB) 2020, pg. 1-10.
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C50. Chen X[g], Akhter N[g], Guo Z[g], Wu T[g], Hou J[g], **Shehu A**, and Cheng J*. *Deep Ranking in Template-free Protein Structure Prediction.* In Proc ACM Conf on Bioinf and Comp Biol (BCB) 2020, pg. 1-10.
[AR: 20%]

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C45. Rajabi Z^g, Uzuner O, and **Shehu A***. *Beyond Binary Sentiments: A Multi-Channel BiLSTM-CNN model for Mutilabel Emotion Classification of Informal Text.* In Proc IEEE Intl Conf on Semantic Computing (ICSC), San Diego, CA, 2020. [AR: 23%]

C44. Tadepalli S^g, Akhter N^g, Barbará D, and **Shehu A***. *Identifying Near-Native Protein Structures via Anomaly Detection.* In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), San Diego, CA, 2019, pg. 30-35.[AR: 19%]

C43. Akhter N^g, Vangara R, Chennupati G, Alexandrov B, Djidjev H, and **Shehu A***. *Non-Negative Matrix Factorization for Selection of Near-Native Protein Tertiary Structures.* In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), San Diego, CA, 2019, pg. 70-73. [AR: 19%]

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C41. Rajabi Z^g, **Shehu A**, and Purohit H*. *User Behavioral Modeling for Fake Information Mitigation on Social Web.* In Proc SBP-BRiMS, Washington, D.C., 2019. [AR: 21%]

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C38. Zaman AB^g and **Shehu A***. *Equipping Decoy Generation Algorithms for Template-free Protein Structure Prediction with Maps of the Protein Conformation Space.* In Proc Intl Conf on Bioinf and Comp Biol (BiCoB), Honolulu, HI 2019, *Finalist for Best Paper Award.* [AR: 40%]

C37. Nasrin Akhter^g, Gopinath Chennupati, Hristo Djidjev, and **Shehu A***. *Improved Decoy Selection via Machine Learning and Ranking.* In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), Las Vegas, Nevada 2018). [AR: 40%]

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C30. Sapin E^p, De Jong KA, and **Shehu A***. *A Novel EA-based Memetic Approach for Efficiently Mapping Complex Fitness Landscapes.* In Proc Genet and Evol Comp Conf (GECCO), Denver, CO, 2016, pg. 85-92. [AR: 40%]

C29. Pandit R^h and **Shehu A***. *A Principled Comparative Analysis of Dimensionality Reduction Techniques on Protein Structure Decoy Data.* In Proc Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2016, pg. 43-48. [AR: 40%]

C28. Maximova T^p, Plaku E*, and **Shehu A***. *Computing Transition Paths in Multiple-Basin Proteins with a Probabilistic Roadmap Algorithm Guided by Structure Data.* In Proc IEEE Intl Conf on Bioinf and Biomed

(BIBM), Washington, D.C., 2015, pg. 35-42.   [AR: 19%]

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C26. Molloy K^g and **Shehu A***. *Interleaving Global and Local Search for Protein Motion Computation.* In Lecture Notes in Computer Science: Bioinformatics Research and Applications, vol. 9096, pg. 175-186 (Proc 11th Intl Symp Bioinf Res & Appl – ISBRA) Norfolk, VA, 2015, vol 9096, pg. 175-186.   [AR: 30%]

C25. Clausen R^g, Sapin E^p, De Jong KA, and **Shehu A***. *Evolution Strategies for Exploring Protein Energy Landscapes.* In Proc Genet and Evol Comp Conf (GECCO), Madrid, Spain, 2014, pg. 217-224.   [AR: 50%]

C24. Veltri D^g, Kamath U, and **Shehu A***. *A Novel Method to Improve Recognition of Antimicrobial Peptides through Distal Sequence-based Features.* In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Belfast, UK, 2014, pg. 371-378 *(Best Student Paper Award).*   [AR: 19%]

C23. Devaurs D, **Shehu A***, Simeon T and Cortes S. *Sampling-based Methods for a Full Characterization of Energy Landscapes of Small Peptides.* In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Belfast, UK, 2014, pg. 37-44.   [AR: 19%]

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C21. Hashmi I^g, Veltri D^g, Kabbani N, and **Shehu A***. *Knowledge-based Search and Multiobjective Filters: Proposed Structural Models of GPCR Dimerization.* In Proc ACM Conf on Bioinf and Comp Biol (BCB), Newport Beach, CA, 2014, pg. 279-288.   [AR: 25%]

C20. Olson, B^g and **Shehu A***. *Multi-Objective Optimization Techniques for Conformational Sampling in Template-Free Protein Structure Prediction.* In Proc Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2014, pg. 1-6.   [AR: 40%]

C19. Molloy, K^g and **Shehu A***. *A Probabilistic Roadmap-based Method to Model Conformational Switching of a Protein Among Many Functionally-relevant Structures.* In Proc Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2014, pg. 1-6 *(finalist for Best Paper Award).*   [AR: 40%]

C18. Randou E, Veltri D^g, and **Shehu A***. *Binary Response Models for Recognition of Antimicrobial Peptides.* In Proc ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C. 2013, pg. 76-85.   [AR: 20%]

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[AR: 20%]

C16. Randou E, Veltri D^g, and **Shehu A***. *Systematic Analysis of Global Features and Model Building for Recognition of Antimicrobial Peptides.* In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), New Orleans, LA, 2013, pg. 1-6.   [AR: 42%]

C15. Molloy K^g, Van JM^u, Barbara D, and **Shehu A***. *Higher-order Representations for Automated Organization of Protein Structure Space.* In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), New Orleans, LA, 2013, pg. 287-294.   [AR: 42%]

C14. Olson B^g, De Jong KA, and **Shehu A***. *Off-Lattice Protein Structure Prediction with Homologous Crossover.* In Proc Genet and Evol Comp Conf (GECCO), Amsterdam, Netherlands, 2013.   [AR: 36%]

C13. Veltri D^g and **Shehu A***. *Physicochemical Determinants of Antimicrobial Activity.* In Proc Intl Conf on Bioinf and Comput Biol, (BICoB), Hawaii, 2013, pg. 1-6.   [AR: 20%]

C12. Hashmi I^g and **Shehu A***. *A Basin Hopping Algorithm for Protein-Protein Docking.* In Proc IEEE Intl Conference on Bioinformatics and Biomedicine (BIBM) 2012, Philadelphia, PA, pg. 466-469.   [AR: 20%]

C11. Molloy K^g and **Shehu A***. *Biased Decoy Sampling to Aid the Selection of Near-Native Protein Conformations.* In Proc ACM Bioinf and Comp Biol (BCB), Orlando, FL, 2012, pg. 131-138.   [AR: 21%]

C10. Olson B^g and **Shehu A***. *Efficient Basin Hopping in the Protein Energy Surface.* In Proc IEEE Conference on Bioinformatics and Biomedicine (BIBM), Philadelphia, PA, 2012, pg. 119-124.   [AR: 20%]

C9. Kamath U^g, Kaers J, **Shehu A** and De Jong KA*. *A Spatial EA Framework for Parallelizing Machine Learning Methods.* In Proc Intl Conf on Parallel Problem Solving From Nature (PPSN), Taormina, Italy, 2012, LNCS vol. 7491, pg. 206-215.   [AR: 47%]

C8. Olson B^g and **Shehu A***. *Populating Local Minima in the Protein Conformational Space.* In Proc IEEE Intl Conference on Bioinformatics and Biomedicine (BIBM), Atlanta, GA, 2011, pg. 114-117.   [AR: 20%]

C7. Kamath U^g, De Jong KA*, and **Shehu A***. *An Evolutionary-based Approach for Feature Generation: Eukaryotic Promoter Recognition.* In Proc IEEE Congress on Evolutionary Computation (CEC), New Orleans, LA, 2011, pg. 277-284.   [AR: 51%]

C6. Olson B^g, Molloy K^g, and **Shehu A***. *Enhancing Sampling of the Conformational Space Near the Protein Native State.* In Proc Intl. Conference on Bio-inspired Models of Network, Information, and Computing Systems (BIONETICS), Boston, MA, 2010, LNICST (Springer), vol. 87, pg. 249-263, *(Best Student Paper Award).*
[AR: 24%]

C5. Kamath U^g, **Shehu A***, and De Jong KA*. *Feature and Kernel Evolution for Recognition of Hypersensitive Sites in DNA Sequences.* In Proc Intl. Conference on Bio-inspired Models of Network, Information, and Computing Systems (BIONETICS), Boston, MA, 2010, LNICST (Springer), vol. 87, pg. 213-238. [AR: 24%]

C4. Kamath U^g, **Shehu A***, and De Jong KA*. *Using Evolutionary Computation to Improve SVM Classification.* In Proc IEEE World Congress on Computational Intelligence (WCCI), Barcelona, Spain, 2010, pg. 1-8.
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C3. Kamath U^g, De Jong KA*, and **Shehu A***. *Selecting Predictive Features for Recognition of Hypersensitive Sites of Regulatory Genomic Sequences with an Evolutionary Algorithm.* In Proc Genet and Evol Comp Conf (GECCO), Portland, Oregon, 2010, pg. 179-186. [AR: 45%]

C2. Richardson SM, Olson B^g, Dymond JS, Burns S, Chandrasegaran S, Boeke JD, **Shehu A**, and Bader JS*. *Automated Design of Assemblable, Modular, Synthetic Chromosomes.* In Proc Lecture Notes in Computer Science: Parallel Processing and Applied Mathematics (PPAM), 2009, vol. 6068, pg. 280-289. [AR: 36%]

C1. **Shehu A***. *An Ab-initio Tree-based Exploration to Enhance Sampling of Low-energy Protein Conformations.* In Proc Robotics: Science and Systems (RSS), 2009, pg. 31-39. [AR: 25%]

Refereed Workshop Publications

W42. Ghaemi S^g, and Rodoshi RT^g, and Shultana S^g, **Shehu A***, and Barbará D*. *From Contrast to Control: Domain Conditioned Masking for Small Molecule Generation of Quaternary Ammonium Compounds.* In Proc Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Philadelphia, PA, 2025, pg. 1-6.

W41. Circi D, Bradley M, Blouir S^g, Wilthan B, Anastasopoulos A, **Shehu A**, Catherine L, and Dhingra B. *Information Extraction from Diverse Charts In Materials Science.* CoLM: LM4Sci Workshop, Montreal, CA, 2025.

W40. Lian Y^g and **Shehu A***. *DyVarMap: An Interpretable, Dynamics-Aware Framework for Missense Variant Classification.* In Proc Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Philadelphia, PA, 2025, pg. 1-6.

W39. Blouir S^g, Watkins C, Blouir Downing C, and **Shehu A***. *SLP Sidekick: Open-Source AI for Speech Therapy with Community-Driven Standards.* First Workshop on Sociotechnical AI Governance: Opportunities and Challenges for HCI, ACM CHI Yokahama, Japan, 2025.

W38. Blouir S^g, Circi D^g, Moldwin A^g, and **Shehu A***. *BirdieDNA: Reward-Based Pre-Training for Genomic Sequence Modeling.* ICLR 2025 Workshop on Machine Learning for Genomics Explorations (ICLR MLGenX), Singapore, 2025.

W37. Kabir A^g, Inan TT^g, Rasmussen K, **Shehu A**, Usheva A, Bishop A, Alexandrov B, and Bhattarai M*. *Scalable DNA Feature Generation and Transcription Factor Binding Prediction via Deep Surrogate Models.* FMs4Bio Workshop at the 39th Annual AAAI Conference on Artificial Intelligence (AAAI), Philadelphia, PA, 2025.

W36. Moldwin A^g and **Shehu A***. *Foundation Models for AI-enabled Biological Design.* FMs4Bio Workshop at the 39th Annual AAAI Conference on Artificial Intelligence (AAAI), Philadelphia, PA, 2025.

W35. Tahmid TT^g, Kabir A^g, Rasmussen K, **Shehu A**, Usheva A, Bishop A, Alexandrov B, and Bhattarai M*. *Efficient High-Throughput DNA Breathing Features Generation Using Jax-EPBD.* FMs4Bio Workshop at the 39th Annual AAAI Conference on Artificial Intelligence (AAAI), Philadelphia, PA, 2025.

W34. Inan TT^g, Liu M, and **Shehu A***. *Optimization Effectiveness versus Generalization Capability of Stochastic Optimization Algorithms for Deep Learning.* Intl Conf on Learning Representations (ICLR) 2024 Workshop on Bridging the Gap Between Practice and Theory in Deep Learning, Vienna, Austria, 2024.

W33. Moldwin A^g, Kabir A^g, and **Shehu A***. *A More Informative and Reproducible Remote Homology Evaluation for Protein Language Models.* LLMs4Bio Workshop at the 38th Annual AAAI Conference on Artificial Intelligence (AAAI), Vancouver, CA, 2024.

W32. Kabir A^g, Moldwin A, and **Shehu A***. *A Comparative Analysis of Transformer-based Protein Language Models for Remote Homology Prediction.* In Proc Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2022, pg. 1-8.

W31. Herceg M^{g*} and **Shehu A***. *Structure- and Energy-based Analysis of Small Molecule Ligand Binding to Steroid Nuclear Receptors.* In Proc Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2022, pg. 1-8.

W30. Rahman T^g, Alam FF^g and **Shehu A***. *Equivariant Encoding based GVAE (EqEn-GVAE) for Protein Ter-*

tiary Structure Generation. In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Las Vegas, Nevada, 2022, pg. 1-8.

W29. Wang Y[u], Ghaemi S[g], Ding A[u], Du Y[u], Pan B[g], Qin M[g], Lin X[g], Petersen AA[g], Leitgeb A[g], Alkhalifa S, Minbiole K, Wuest WM, Zhao L, and **Shehu A**[*]. *Generation and Characterization of Quaternary Ammonium Compounds via Deep Learning.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Las Vegas, Nevada, 2022, pg. 1-8.

W28. Pan B[g], Wang Y[u], Lin X[g], Qin M[g], Du Y[u], Ghaemi S[g], Ding A[u], Wang S[g], Alkhalifa S, Minbiole K, Wuest WM, Petersen AA[g], Leitgeb A[g], **Shehu A**, and Zhao L[*]. *Property-Controllable Generation of Quaternary Ammonium Compounds.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Las Vegas, Nevada, 2022, pg. 1-8.

W27. Pan B[g], Wang Y[u], Lin X[g], Du Y[u], Ghaemi S[g], Ding A[u], Wang S[g], **Shehu A**, and Zhao L[*]. *Property-Controllable Generation of Quaternary Ammonium Compounds.* In Proc ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) Workshop on Deep Learning on Graphs: Methods and Applications (DLG-KDD'22), Washington, D.C., 2022.

W26. Kamranfar P[g], Lattanzi D, **Shehu A**, and Barbara D[*]. *Multiple Instance Learning for Detecting Anomalies over Sequential Real-World Datasets.* In Proc ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) Workshop on Anomaly and Novelty Detection (ANDEA) , Washington, D.C., 2022.

W25. Du Y[u], Guo X, **Shehu A**, and Zhao L[*]. *Interpretable Molecular Graph Generation via Monotonic Constraints.* In Proc Neural Information Processing Systems (NeurIPS) Workshops: ML4Molecules, Virtual, 2021.

W24. Alam FF[g] and **Shehu A**[*]. *Generating Physically-Realistic Tertiary Protein Structures with Deep Latent Variable Models Learning Over Experimentally-available Structures.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Virtual, 2021, pg. 1-8.

W23. Kabir KL[g], Ma B, Nussinov R, and **Shehu A**[*]. *Antigen Binding Reshapes Antibody Energy Landscape and Conformation Dynamics.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Virtual, 2021, pg. 1-8.

W22. Du Y[u], Guo X[g], Zhao L[*], and **Shehu A**[*]. *Interpretable Molecule Generation via Disentanglement Learning.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2020, pg. 1-8.

W21. Du Y[u], Kabir A[g], Zhao L[*], and **Shehu A**[*]. *From Interatomic Distances to Protein Tertiary Structures with a Deep Convolutional Neural Network.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2020, pg. 1-8.

W20. Zaman AB[g], Kamranfar P[g], Domeniconi C, and **Shehu A**[*]. *Decoy Ensemble Reduction in Template-free Protein Structure Prediction.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Buffalo, NY 2019, pg. 562-567.

W19. Alam FF[g], Rahman [g], and **Shehu A**[*]. *Learning Reduced Latent Representations of Protein Structure Data.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Buffalo, NY 2019, pg. 592-597.

W18. Dua M[g], Veltri D, Bishop B, and **Shehu A**[*]. *Guiding Exploration of Antimicrobial Peptide Space with a Deep Neural Network.* IEEE BIBM Workshops: Artificial Intelligence Techniques for BioMedicine and HealthCare (AIBH), Madrid, Spain 2018, pg. 2082-2087.

W17. Hassan L[g], Rajabi Z[g], Akhter N[g], and **Shehu A**[*]. *Community Detection for Decoy Selection in Template-free Protein Structure Prediction.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D.C. 2018, pg. 621-625.

W16. Almsned F[g], Gogovi G[g], Bracci[g], Kehn-Hall K, Blaisten-Barojas E, and **Shehu A**[*]. *Modeling the Tertiary Structure of a Multi-domain Protein.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D.C. 2018, pg. 615-620.

W15. Sapin E[p], De Jong KA, and **Shehu A**[*]. *Evolving Conformation Paths to Model Protein Structural Transitions.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Boston, MA, 2017, pg. 673-678.

W14. Qiao W[*], Maximova T[p], Plaku E, and **Shehu A**[*]. *Statistical Analysis of Computed Energy Landscapes to Understand Dysfunction in Pathogenic Protein Variants.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Boston, MA, 2017, pg. 679-684.

W13. Sapin K[p], De Jong KA, and **Shehu A**[*]. *An Evolutionary Algorithm to Model Structural Excursions of a Protein.* In Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Berlin, Germany, 2017, pg. 1669-1673.

W12. Sapin K[p], De Jong KA, and **Shehu A**[*]. *Path-based Guidance of an Evolutionary Algorithm in Mapping a Fitness Landscape and its Connectivity.* In Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Workshops, Denver, CO, 2016, pg. 1293-1298.

W11. Sapin K[p], De Jong KA, and **Shehu A**[*]. *Mapping Multiple Minima in Protein Energy Landscapes with*

Evolutionary Algorithms. In Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Workshops, Madrid, Spain, 2015, pg. 923-927.

W10. Molloy K^g, Clausen R^g, and **Shehu A***. *On the Stochastic Roadmap to Model Functionally-related Structural Transitions in Wildtype and Variant Proteins.* In Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems - Robotics: Science and Systems (RSS) Workshops, Berkeley, CA, 2014, pg. 1-6.

W9. **Shehu A*** and De Jong KA. *Memetic, Multi-Objective, Off-Lattice, and Multiscale Evolutionary Algorithms for De-novo and Guided Protein Structure Modeling.* In Workshop on Natural Computing for Protein Structure Prediction - Intl Conf on Parallel Problem Solving from nature (PPSN) Workshops, Ljubljana, Slovenia, 2014, pg. 1-2.

W8. Clausen R^g and **Shehu A***. *Exploring the Structure Space of Wildtype Ras Guided by Experimental Data.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D. C., 2013, pg. 757-764.

W7. Hashmi I^g and **Shehu A***. *Informatics-driven Protein-protein Docking.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D. C., 2013, pg. 772-779.

W6. Olson B^g and **Shehu A***. *An Evolutionary Search Algorithm to Guide Stochastic Search for Near-native Protein Conformations with Multiobjective Analysis.* In Workshop on Artificial Intelligence and Robotics Methods in Computational Biology - Intl Conf of Association for Advancement of Artificial Intelligence (AAAI) Workshop, Bellevue, WA, 2013, pg. 32-37.

W5. Molloy M^g and **Shehu A***. *A Robotics-inspired Method to Sample Conformational Paths Connecting Known Functionally-relevant Structures in Protein Systems.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Philadelphia, PA, 2012, pg. 56-63.   [AR: 33%]

W4. Saleh S^u, Olson B^g, and **Shehu A***. *A Population-based Evolutionary Algorithm for Sampling Minima in the Protein Energy Surface.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Philadelphia, PA, 2012, pg. 48-55.   [AR: 33%]

W3. Olson B^g, Hendi, S-F^g, and **Shehu A***. *Protein Conformational Search with Geometric Projections.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 366-373.
[AR: 40%]

W2. Akbal B, Hashmi I^g, **Shehu A**, and Haspel N*. *Refinement of Docked Protein Complex Structures Using Evolutionary Traces.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 400-404.   [AR: 40%]

W1. Hashmi I^g, Akbal B, Haspel N, and **Shehu A***. *Protein Docking with Information on Evolutionary Conserved Interfaces.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 358-365.   [AR: 40%]

Book Chapters

B7. Kabir A^g and **Shehu A***. *Graph Neural Networks for Predicting Protein Function, Activity, and Molecular Interactions.* In Graph Neural Networks on Proteins and DNA. Springer Series on Graph Neural Networks: Foundations, Frontiers, and Applications, first edition, (Editors: Wu, L., Cui, P., Pei, J., and Zhao, L.), 2021.

B6. Akhter N^g, Hassan L^g, Rajabi Z^g, Barbará D, and **Shehu A***. *Learning Organizations of Protein Energy Landscapes: An Application on Decoy Selection in Template-Free Protein Structure Prediction.* In Methods in Molecular Biology: Protein Supersecondary Structure (Springer), first edition, (Editor: Kister, A.), 2018.

B5. Kamath U, Domeniconi C, **Shehu A**, and Kenneth De Jong*. *EML: A Scalable, Transparent Meta-Learning Paradigm for Big Data Applications.* In Intelligent Systems Reference Library: Innovations in Big Data Mining and Embedded Knowledge (Springer), first edition, (Editor: Anna Esposito, Antonietta M. Esposito, and Lakhmi C. Jain), 2018.

B4. **Shehu A***, Barbará D, and Molloy K. *A Survey of Computational Methods for Protein Function Prediction.* In Big Data Analytics in Genomics (Springer), first edition, (Editors: Wong, KC), 2016.

B3. **Shehu A** *A Review of Evolutionary Algorithms for Computing Functional Conformations of Protein Molecules.* In Computer-Aided Drug Discovery (Springer Methods in Pharmacology and Toxicology Series), first edition, (Editors: Zhang W), 2015.

B2. **Shehu A** *Probabilistic Search and Optimization for Protein Energy Landscapes.* In Handbook of Computational Molecular Biology, Chapman & Hall/CRC Computer & Information Series, 2nd edition (Editors: Aluru S and Singh M), 2013.

B1. **Shehu A**. *Conformational Search for the Protein Native State.* In Protein Structure Prediction: Method and Algorithms, Wiley Book Series on Bioinformatics, 2009.

F4. Lightly-Refereed Publications

Summary

Abstracts are typically 1-2 paragraph submissions that are lightly reviewed and accepted either as poster or oral presentations at conferences and workshops; in the case of oral presentations, such as at 3DSIG, the review process is more rigorous. Extended abstracts are typically viewed as condensed manuscript submissions of 1-3 pages and are also more rigorously reviewed. All extended abstracts listed in this CV are indexed by ACM or IEEE and assigned their own doi.

Extended Abstracts, Abstracts, and Posters

78. Blouir S[g], Acharya P[g], Anastasopoulos A, and **Shehu A***. *Fusing LLaMa with State-Space Models: Efficient Contextualization via Parameter-free State-Space Cross-Attention.* MASC-SLL", Penn State University, April 05, 2025.

77. Kabir A[g] and **Shehu A***. *Foundation Models for Transcription Factor Binding Site Prediction.* Children's Brain Tumor Network Summit, Arlington, VA, October, 2024.

76. Moldwin A[g], Kabir A[g], and **Shehu A***. *Protein Language Models in the Twilight Zone of Protein Sequence Homology.* Children's Brain Tumor Network Summit, Arlington, VA, October, 2024.

75. Peterson AA[g], Leitgeb A[g], Alkhalifa S, Zhao L, **Shehu A**, Wuest WM, and Minbiole K*. *Incorporation of Machine Learning Strategies in the Development of Quaternary Ammonium Compounds.* American Chemical Society National Meeting, Indianapolis, IN, March, 2023.

74. Herceg M[g], Brown M, and **Shehu A***. *Computational evidence of BRCA1-NC3 receptor interaction and druggability analysis in BRCA1-related oncogenesis.* American Society of Human Genetics Symposium, Virtual, October, 2021 (Poster).

73. Liang Y[g], Bodian D, and **Shehu A***. *3D conformation analysis of the FGFR2 kinase domain with disease-associated mutations reveals novel features that correlate with clinical presentation.* American Society of Human Genetics Symposium, Virtual, October, 2021 (Poster).

72. Dua M[g], Veltri D, Bishop B, and **Shehu A***. *Exploring the Space of Antimicrobial Peptides Guided by a Deep Learning Model.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

71. Kabir, LK[g], Akhter N[g] and **Shehu A***. *Unsupervised Learning of Conformational States Present in Molecular Dynamics Simulation Data for Summarization of Equilibrium Conformational Dynamics.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

70. Akhter N[g] and **Shehu A***. *Unsupervised Learning for Decoy Selection in Protein Structure Prediction.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

69. Zaman AB[g] and **Shehu A***. *A Multi-Objective Stochastic Optimization Approach for Decoy Generation in Template-Free Protein Structure Prediction.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

68. Roychoudhoury S[h] and **Shehu A***. *Systematic Study of Different Design Decisions in Markov Model-based Analysis of Molecular Structure Data.* (extended abstract and poster presentation, pg. 508-509). ACM BCB. Washington, DC, August 29 - September 01, 2018. (*Honorable Mention*)

67 Molloy K, Akhter N[g], and **Shehu A***. ACM-BCB '18 Tutorial: *Modeling Macromolecular Structures and Motions: Computational Methods for Sampling and Analysis of Energy Landscapes.* (abstract and tutorial presentation, pg. 554). ACM BCB. Washington, DC, August 29 - September 01, 2018.

66. **Shehu A***. *Reconstruction and Mining of Energy Landscapes of Ras Variants.* Ras Initiative Symposium. Frederick National Laboratory for Cancer Research, National Cancer Institute, Frederick, MD, December 6-8, 2017. (Abstract and Poster).

65. **Shehu A***. *Guiding Stochastic Optimization Algorithms with Experimental Data to Model Protein Energy landscapes and Structural Transitions.* Thematic Meeting of the Biophysical Society: Conformational Ensembles from Experimental Data and Computer Simulations. Berlin, Germany, August 25-29, 2017. (Abstract and Poster).

64. Molloy K, Morris D[g], and **Shehu A***. "ACM-BCB '17 Tutorial: *Robotics-inspired Algorithms for Modeling Protein Structures and Motions.* (abstract and tutorial presentation, pg. 628). ACM BCB. Boston, MA, August 20-23, 2017.

63. Maximova T[p], Qiao W, Plaku E, Plaku E, Mattos C, Ma B, Nussinov R, and **Shehu A***. *From Mutations to Mechanisms and Dysfunction via Computation and Mining of Protein Energy Landscapes.* 3DSIG at Intelligent Systems for Molecular Biology (ISMB). Prague, Czech Republic, July 22-23, 2017. (Abstract and Oral Presentation).

62. Sapin E[p], De Jong KA, and **Shehu A***. *Evolutionary Search for Paths on Protein Energy Landscapes.* ACM

GECCO, Berlin, Germany, July 15-19, 2017. (Two-page poster paper).

61. **Shehu A**[*]. *Big, Molecular Structure Data Demand Automated Landscape Analysis.* UC Davis RTG Statistical Sciences Symposium: Geometry, Statistics, and Data Analysis. Davis, California, May 19-20, 2017. (Poster and Abstract).

60. Maximova T[p], Plaku E, and **Shehu A**[*]. *Method for Extended Sampling and Transition Paths Prediction with Probabilistic Roadmap Algorithm.* 3DSig, Intelligent Systems for Molecular Biology (ISMB) Orlando, Florida, July 2016 (Poster and Extended Abstract). *Outstanding Research Presentation Award*).

59. Marquez M, McDermott-Roe C[*], Bukowy J, Kolander K, Kuo J, Maximova T[p], **Shehu A**, Benjamin I, and Geurts A. *Modeling BAG3-associated cardiomyocyte dysfunction via genome editing in induced pluripotent stem cells.* Keystone Symposia on Molecular and Cellular Biology: Heart Failure: Genetics, Genomics and Epigenetics, Snowbird Resort, Snowbird, Utah, April 2016 (Poster and Abstract).

58. McDermott-Roe C[*], Mitzefelt K, Marquez M, Grzybowski M, Bukowy J, Maximova T[p], **Shehu A**, Benjamin I, and Geurts A. *Modeling BAG3-associated cardiomyocyte dysfunction via genome editing in induced pluripotent stem cells.* CRISPR Precision Gene Editing Congress, Boston, Massachussetts, February 2016 (Poster and Abstract).

57. Mazyar K[u], Hashmi I[g], Neil A, and **Shehu A**[*]. *Platform to Support Intensive Webserver Computations on Argo.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration, Fairfax, VA, April 2015 (Poster).

56. Songyue H[u] and **Shehu A**[*]. *A new Distance Function for Protein Structures for the Decoy Selection Problem in De-novo Structure Prediction.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration, Fairfax, VA, April 2015 (Poster).

55. Clausen R[g], **Shehu A**[*], Ma B, and Nussinov R. *A Novel Evolutionary Algorithm to Model Energy Landscapes of Wildtype and Variant Sequences of H-Ras.* Biophysical Society Meeting, Baltimore, MD, February, 2015 (Poster).

54. Clausen R[g], **Shehu A**[*], Ma B, and Nussinov R. *Mapping the Structure Space of the Ras Protein using a Novel Hybrid Evolutionary Algorithm.* NIH Summer Poster Day, Fredericks, MD, July, 2014 (Poster).

53. Van MJ[u], Namazi M[u], Xiang R[u], Blaisten-Barojas E[*], and **Shehu A**[*]. *Structural Analysis and Dynamics of the Met-Enkephalin Peptide.* American Chemical Society (ACS) Undergraduate Research Poster Session, Charlottesville, VA, April 2014 (Poster).

52. Pilapitiya H[u], Kabbani N[*], and **Shehu A**[*]. *Modeling Binding of Amyloid beta-42 Peptide to the Alpha 7 Nicotinic Receptor.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

51. Van MJ[u], Namazi M[u], Xiang R[u], Blaisten-Barojas E[*], and **Shehu A**[*]. *Conformational Sampling and Principal Component Analysis of the Met-Enkephalin Peptide.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

50. Namazi M[u], Van MJR[u], Xiang R[u], **Shehu A**[*] and Blaisten-Barojas E[*]. *Molecular Dynamics Simulation of the Met-Enkephalin Peptide with Explicit Solvent.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

49. Xiang R[u], Van MJR[u], Namazi M[u], Blaisten-Barojas E[*], and **Shehu A**[*]. *A Clustering Algorithm for Molecular Structures: Application on the Met-Enkephalin Peptide.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

48. Clausen R[g] and **Shehu A**[*]. *A PCA-guided Search Algorithm to Probe the Conformational Space of the Ras Protein.* ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C., September 2013 (Extended Abstract and Poster).

47. Hashmi I[g] and **Shehu A**[*]. *Protein-protein Docking using Information from Native Interaction Sites.* ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C., September 2013 (Extended Abstract and Poster).

46. Olson B[g] and **Shehu A**[*]. *A Multi-objective Guided Evolutionary Search Algorithm for Sampling Near-native Protein Conformations.* Workshop on Artificial Intelligence and Robotics Methods for Computational Biology - Conf on Association for Advancement of Artificial Intelligence Workshop, Bellevue, WA, July 2013 (Poster).

45. Randou EG, Veltri D[g], and **Shehu A**[*]. *Towards Classification and Virtual Screening of Antimicrobial Peptides with Regression-based Binary Response Models.* Nonclinical Biostatistics Conference (NCB), Villanova University, PA, 2013 (Abstract and Oral Presentation).

44 Molloy K[g], Van JM[u], Barbara D, and **Shehu A**[*]. *Higher-order Representations for Automated Organization of Protein Structure Space.* Celebration of Undergraduate Student Scholarship, George Mason University,

Fairfax, VA, May 2013 (Poster).

43. Saleh S^u, Olson B^g, and **Shehu A***. *An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.* National Council of Undergraduate Research (NCUR), University of Wisconsin-La Crosse, La Crosse, WI, 2013 (Abstract and Poster).

42. Shehu A. *Probabilistic Methods for Modeling Structures and Motions of Protein Systems.* NFS Grants Conference, Fairfax, VA, 2012 (Poster).

41. Bohidar N^h and **Shehu A***. *From Coarse-grained Conformations to Motion Pathways in Proteins.* Thomas Jefferson Senior Research Day, Alexandria, Virginia, April 2013 (Poster).

40. Reinstadler B^u, Van JM^g, and **Shehu A***. *Supersecondary Structure Motifs and De Novo Protein Structure Prediction.*Grace Hopper Conference Celebration of Women in Computing, Baltimore, MD, 2012 (Abstract and Poster).

39. Saleh S^u, Olson B^u and **Shehu A***. *An evolutionary framework to sample near-native protein conformations.* CSBW at IEEE BIBM Workshops (BIBM-W), pg. 933. (Extended Abstract and Poster).

38. Veltri D* and **Shehu A***. *Physico-chemical features for recognition of antimicrobial peptides.* CSBW at IEEE BIBM Workshops (BIBM-W), pg. 942. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

37. Olson B^g and **Shehu A***. *An evolutionary search framework to efficiently sample local minima in the protein conformational space.* ACM BCB, pg. 590. Orlando, FL, 2012 (Extended Abstract and Poster).

36. Hashmi I^g and **Shehu A***. *Sampling low-energy protein-protein configurations with basin hopping.* IEEE BIBM, pg. 947. Philadelphia, PA, October 4-7, 2012. (Extended Abstract and Poster, <u>*Best Poster Award*</u>).

35. Olson B^g and **Shehu A***. *Jumping low, jumping high: Controlling hopping in the protein energy surface.* IEEE BIBM, pg. 946. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

34. Molloy K^g and **Shehu A***. *A tree-based search to bias sampling of protein decoy conformations.* IEEE BIBM, pg. 978. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

33. Molloy K^g and **Shehu A***. *Mapping conformational pathways between known functional protein states.* CSBW at IEEE BIBM Workshops (BIBM-W), pg. 971. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

32. Jordan S^u and **Shehu A***. *Refinement of Coarse-grained Near-native Protein Conformations Using AMBER FF99SB Force Field.* Aspiring Scientist Summer Internship Program (ASSIP) Poster Presentations, Manassas, Virginia, Summer 2012 (Poster).

31. Saleh S^u, Olson B^g, and **Shehu A***. *An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.* Celebration of Student Scholarship, Fairfax, VA, May 2012 (Poster).

30. Saleh S^u, Olson B^g, and **Shehu A***. *Revisiting Evolutionary Search for Effective Sampling of Near-native Conformations in the Protein Conformational Space.* Virginia Academy of Sciences, Norfolk, VA, May 2012 (Abstract and Poster).

29. Saleh S^u and **Shehu A***. *An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.* College of Science Symposium, George Mason University, Fairfax, VA, May 2012 (Poster).

28. Olson B^g and **Shehu A***. *A Basin Hopping Probabilistic Search Framework to Efficiently Sample Local Minima in the Protein Conformational Space.* 26th Annual Meeting of the Protein Society, San Diego, CA, 2012 (Abstract and Poster).

27. Olson B^g and **Shehu A***. *A Basin Hopping Probabilistic Search Framework to Efficiently Sample Local Minima in the Protein Conformational Space.* Intelligent Systems for Molecular Biology (ISMB) Student Council, Long Beach, CA, 2012 (Abstract and Poster).

26. Molloy K^g and **Shehu A***. *Assembly of Low-Energy Protein Conformations with Heterogeneous Fragments.* IEEE BIBM, pg. 991-993. Atlanta, GA, November 12-15, 2012 (Extended Abstract and Poster).

25. Olson B^g and **Shehu A***. *Mapping the Protein Conformational Landscape with Adaptive Probabilistic Search.* 55th Annual Meeting of the Biophysical Society, Baltimore, Maryland, 2011 (Abstract and Poster).

24 : Hashmi I*, Akbal-Delibas B, Haspel N, and **Shehu, A***. *Protein Docking with Information on Evolutionary Conserved Interfaces.* Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshop, Atlanta, GA, November, 2011 (Abstract and Poster).

23 Olson B^g and **Shehu, A***. *Local Minima Hopping Along the Protein Energy Surface.* IEEE Intl Conf on Biomed and Bioinf (BIBM), Atlanta, GA, November, 2011 (Abstract and Poster).

22. Richardson SM, Olson B^g, Dymond JS, Burns R, Chandrasegaran S, Boeke JD, **Shehu A**, and Bader JS*. *Automated Design of Assemblable, Modular, Synthetic Chromosomes.* Annual RECOMB Satellite Meeting on Regulatory Genomics and Systems Biology, Boston, MA, 2009 (Abstract and Oral Presentation).

21. Chung R^u, Jamil B^u, and **Shehu A***. *A Metropolis Monte Carlo Algorithm to compute Low-energy Structures of an RNA chain.* Grace Hopper Conference Celebration of Women in Computing, Tucson, Arizona, 2009 (Abstract and Poster).

20. Mostaghim A^u, Veltri D^g, Majul A^g, and **Shehu A***. Aspiring Scientist Summer Internship Program (ASSIP) Poster Presentations, Manassas, Virginia, 2009 (Poster).

19. Miles C^g and **Shehu A***. *Computing Symmetric HomoOligomeric Structures.* Intl Conf on Intelligent Systems for Molecular Biology & European Conf on Computational Biology (ISMB-EECB), Stockholm, Sweden, 2009 (Abstract and Poster).

18-1. These posters were the result of Shehu's research as a graduate and undergraduate student and can be found on the lab's website.

F5. Other Selected Publications and Products

Other Publications

23. **Shehu A***, Ababu A, Akbary A, Allen G, Baig A, Battle T, Beall E, Byrom C, Dean M, Demarco K, Douglass E, Granados L, Hantush L, Hay A, Hay E, Jackson C, Jang J, Jones C, Li Q, Lopez A, Massimo L, McMullin G, Mendoza Maldonado A, Mirza E, Muddasar H, Nuwayhid S, Pak B, Petty A, Rancourt D, Rodriguez L, Rogers C, Schiek J, Seok T, Sethi A, Vitela G, Williams W, Yetukuri J. *Can Consumer Chatbots Reason? A Student-Led Field Experiment Embedded in an "AI-for-All" Undergraduate Course.* arXiv:2601.04225, 2025. https://arxiv.org/abs/2601.04225.

22. Moldwin A and **Shehu A***. *How Much Does Protein Structure Really Help? A Case Study in Mutation-Induced Stability Prediction.* bioRxiv 10.64898/2025.12.22.694225, 2025. https://www.biorxiv.org/content/10.64898/2025.12.22.694225v1.

21. **Shehu A***. *Cheap Intelligence: The New GenAI Investment Thesis.* https://perspectives.opulentia.vc/cheap-intelligence-the-new-genai-investment-thesis/

19. **Shehu A*** and Padmanabhan Seshaiyer. *Reference Guide on Integrating Artificial Intelligence into Virginia Education,* https://www.schev.edu/Home/Components/News/News/688/16, September 18, 2025.

18. **Shehu A*** and Acton S. *An Introduction to Artificial Intelligence ,* https://vasem.org/wp-content/uploads/2025/08/VASEM_AI_WhitePaper-2025.pdf, August 18, 2025.

17. Lu Y, **Shehu A***, and Lattanzi, D*. *Accounting for Work Zone Disruptions in Traffic Flow Forecasting.* arXiv 2407.11407 , 2024.

16. Inan TT and **Shehu A***. *Beyond Single-Model Views for Deep Learning: Optimization versus Generalizability of Stochastic Optimization Algorithms.* aRxiv 2403.00574, 2024.

15. Kabir A*, Bhattarai M, Rasmussen K, **Shehu A**, Bishop AR, Alexandrov B, and Usheva A*. *Advancing Transcription Factor Binding Site Prediction Using DNA Breathing Dynamics and Sequence Transformers via Cross Attention.* bioRxiv 10.1101/2024.01.16.575935v2, 2024.

14. Kabir A* and **Shehu A***. *GOProFormer: A Multi-modal Transformer Method for Gene Ontology Protein Function Prediction.* bioRxiv 10.1101/2022.10.20.513033, 2022.

13. Kabir A* and **Shehu A***. *Transformer Neural Networks Attending to Both Sequence and Structure for Protein Prediction Tasks.* arXiv 2206.11057, 2022.

12. Qiao W* and **Shehu A***. *Space Partitioning and Regression Mode Seeking via a Mean-Shift-Inspired Algorithm.* arXiv 2104.10103, 2021.

11. Lu Y[g], Kamranfar P[g], and **Shehu A***. *Traffic Flow Forecasting with Maintenance Downtime via Multi-Channel Attention-Based Spatio-Temporal Graph Convolutional Networks.* arXiv 2110.01535, 2021.

10. Guo X[g], Du Y[u], Tadepalli S[g], Zhao L, and **Shehu A***. *Generating Tertiary Protein Structures via an Interpretative Variational Autoencoder.* arXiv 2004.07119, 2021.

9. Molloy K, Plaku E, and **Shehu A***. *ROMEO: A Plug-and-play Software Platform of Robotics-inspired Algorithms for Modeling Biomolecular Structures and Motions.* arXiv 1905.08331, 2019.

8. **Shehu A***. *Investing in Our Undergraduate Students.* George Mason Review, April 26, 2019.

7. **Shehu A***. *Will China surpass the US in AI technology? Mason experts weigh in.* The George, April 26, 2019.

6. **Shehu A***. *Computer Scientist in Profile: Yang Zhang.* ACM SIGBIO Record 4(2), 2, 2014.

5. **Shehu A***. *Computer Scientist in Profile: Bruce Donald.* ACM SIGBIO Record 4(1), 5-7, 2014.

4. **Shehu A***. *Computational Biologist in Profile: Ruth Nussinov.* ACM SIGBIO Record 3(3), 12-14, 2013.

3. **Shehu A***. *Computer Scientist in Profile: Mona Singh.* ACM SIGBIO Record 3(1), 26-27, 2013.

2. Veltri D[g] and **Shehu A***. *Elucidating Activity-related Physico-chemical Features in Antimicrobial Peptides.* Technical Report, GMU-CS-TR-2012-6, 2012.

1. Miles C[g], Olson B[g], and **Shehu A***. *Geometry-based Computation of Symmetric Homo-oligomeric Protein Complexes.* Technical Report, GMU-CS-TR-2009-2, 2009.

Software

A complete and up-to-date list can be found in our github page at https://github.com/amarda-shehu.

15. GOProFormer: A Multi-Modal Transformer Method for Gene Ontology Protein Function Prediction. Anowarul Kabir and Amarda Shehu. This work has appeared in Biomolecules 12(11):1709, 2022. Code and pre-trained model are available at https://github.com/amarda-shehu/GoProFormer.

14. Generating Tertiary Protein Structures via Interpretable Graph Variational Autoencoders. Xiaojie Guo, Yuanqi Du, Sivani Tadepalli, Liang Zhao, and Amarda Shehu. This work has appeared in Bioinformatics Advances 2021. Code is available at https://github.com/amarda-shehu/CO-VAE.

13. Generative Adversarial Learning of Protein Tertiary Structures. Taseef Rahman, Yuanqi Du, Liang Zhao, and Amarda Shehu. This work has appeared in Molecules 2021. Data and selected trained models are publicly available through IEEE Dataport (ieee-dataport.org) under DOI 10.21227/m8sa-cz14, 2021

12. ROMEO, Object-Oriented, Plug-n-Play Robotics-Inspired Protein Modeling, 2017

11. AMPScreen: Antimicrobial Recognition and Genome-wide Screening, 2016

10. SIfTER: A Structure-guided Memetic, Cellular, and Multiscale Evolutionary Algorithm for Mapping Protein Conformation Spaces, 2015

9. EFC-FCBF: Framework for Feature Construction and Selection for Improved Recognition of Antimicrobial Peptides, 2014

8. HEA-PSP: A Hybrid Evolutionary Search Framework with Various Crossover Implementations for Ab-initio Protein Structre Prediction, 2014

7. EFFECT: Framework for Automated Construction and Extraction of Features for Classification of Biological Sequences, 2013

6. Binary Response Models for Recognition of Antimicrobial Peptides, 2013

5. Statistical Model Building for Antimicrobial Peptide Recognition, 2013

4. Novel features for Antimicrobial Peptide Recognition, 2013

3. Spatial EA Framework for Parallel Machine Learning, 2012

2. An Evolutionary Algorithm For Feature Generation from Sequence Data, 2012

1. An Evolutionary Algorithm For SVM Kernel Optimization, 2011

F6. Invited Talks, Keynotes, and Public Engagement

Invited Talks and Keynotes

108. *Choosing the Future Together: AI Innovation, Community, and Commitment.* Opening Keynote, Faculty and Staff Enrichment Day, George Mason University, Fairfax, Virginia, October 16, 2025.

107. *AI Innovation in Teaching and Learning.* Opening Keynote, Innovations in Teaching and Learning Conference, George Mason University, Fairfax, Virginia, September 26, 2025.

106. *Emerging Technologies and AI Needs in Small Businesses.* Seminar, The Center for AI Innovation and Economic Competitiveness (CAIIEC), George Mason University, Arlington, Virginia, September 19, 2025.

105. *A Public R1 University as an AI Innovation Nexus.* Invited Talk, Micron AI Week, Micron, Virginia, September 16, 2025.

104. *AI for Predictable Bioengineering: From Generation Hype to Functional Understanding.* Invited Presentation, National Academies Workshop Session on Transformative Science & Technology for the Department of Defense: Synthetic Biology for Biomanufacturing and Predictable Engineering, July 01, 2025.

103. *George Mason University AI² Nexus.* Invited Webinar, International Federation of Engineering Education Societies and the Global Engineering Deans Council, June 25, 2025.

102. *Pioneering AI Innovation in Virginia.* Invited Talk, George Mason University SciTech Campus Advisory Board, Manassas, VA, June 12, 2025.

101. *Not for Scale but for (Biological) Discovery: Small(ish) AI.* Invited Talk, Salishan Conference on High Speed Computing, Salishan, OR, April 23, 2025.

100. *Guest Lecture on AI, Biotech, and Health Security.* Johns Hopkins School of Advanced International Studies (SAIS), Washington, D.C, April 7, 2025.

99. *AI for Discovery, Not Just Scale: Purpose-Built Models in Science.* 2025 AI Expo, Oak Ridge National Laboratory, Oak Ridge, TN, April 2, 2025.

98. *Mason: A Nexus of AI Innovation.* Research Committee Report, Board of Visitors, Fairfax, VA, February 27, 2025.

97. *Mason AI Rising.* Guest Lecture, Women in Tech & Women of Color in STEM, Fairfax, VA, February 12, 2025.

96. *Ethics and AI in Public Administration.* Guest Lecture, PUAD 700 (Ethics for Public Administration), Arlington, VA, October 10, 2024.

95. *AI as the Fourth Industrial Revolution -What's Next?* Invited Talk, The Council of State Governments (CSG) Southern Office AI Policy Masterclass, Alexandria VA, September 19, 2024.

94. *Partnering to Disentangle Aging and Menopause.* Invited Talk, NSF-NIH Workshop on Using Artificial Intelligence to Better Understand Menopause, Alexandria VA, September 04-05, 2024.

93. *Enabling and Accelerating Scientific Discovery with Generative AI.* Invited Seminar, Lucy Family Institute for Data and Society, Notre Dame, April 03, 2024.

92. *GenAI In Education.* Masterclass, Gen Next Education, KCG College of Technology, Chennai, January 25, 2024.

91. *Of Small Molecules, Large Molecules, AI, and Generative AI.* Invited Seminar, Center for Genetic Medicine, Children's National Hospital, January 19, 2024.

90. *Artificial Intelligence in the Age of Large Language Models.* Invited Talk, Vienna Area Branch of AAUW and the Patrick Henry Library of Vienna, January 06, 2024.

89. *AI Redux: Opportunities and Dangers Ahead.* Invited Talk, Carlisle Towers, November 05, 2023.

88. *AI & ML Beyond ChatGTP: From Education to Training and Careers in our AI-powered Digital Society.* Masterclass, Gen Next Education, October 20, 2023.

87. *Artificial Intelligence after ChatGTP.* Invited Talk, George Mason Regional Library, Fairfax, VA, September 05, 2023.

86. *How Can Artificial Intelligence (AI) Really Improve Our Lives?* Invited Talk, Prince William Chamber of Commerce Business Series, VA, May 09, 2023.

85. *What Can Artificial Intelligence Tell Us About American Grand Strategy?* Session on Implications of Artificial Intelligence for Global Politics, International Studies Association (ISA) Annual Convention, Montreal, Canada, March 17, 2023 (with M Hunzeker).

84. *The Institutional Determinants of National Artificial Intelligence Infrastructures, Session on Implications of Artificial Intelligence for Global Politics.* International Studies Association (ISA) Annual Convention, Montreal, Canada, March 17, 2023 (with JP Singh).

83. *Are ChatBots ready for Business?* Dell Perspectives, February 01, 2023.

82. *Representation Learning from Genotypes to Phenotypes: Linking Chemical and Biological Space in Small Molecules and Macromolecules.* Keynote, IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM), Las Vegas, NV, December 07, 2022.

81. *AI for Human Biology and Health.* Radio Interview: A Structure Prediction Miracle, With Good Reason, WAMU 88.5FM, December 05, 2022.

80. *Digital Innovation for Digital Therapeutics.* Keynote, International Symposium on Digital Therapeutics, George Mason University, Arlington, VA, November 09, 2022.

79. *AI For Small and Large Molecules: From Foundational Insight to Understanding and Discoveries.* Keynote, 2022 Interdisciplinary Research Fall Forum, The Ohio State University, Columbus, OH, November 08, 2022.

78. *Artificial Intelligence (AI): How did we Get Here, What is Here, and Where we are Heading.* Invited Talk, National Leadership Council, Middleburg, VA, October 29, 2022.

77. *AI and our Digital Society.* Invited Talk, Science Tap Program, Loudon County Public Library, VA, October 06, 2022.

76. *Digital Innovation For Good.* IDIA Presentation, George Mason University Board of Visitors Research Committee Report, Fairfax, VA, September 29, 2022.

75. *The Cultural, Economic, and Institutional Determinants of AI Infrastructures and theirConsequences in Global Contexts.* PI Meeting Presentation, DoD Trust and Influence Program, VA, September 15, 2022.

74. *Common Attributes of Responsive Proposals.* Invited Talk, 30th Conference for Intelligent Systems in Molecular Biology (ISMB), NIH-NSF Smart Health Program Special Track, Madison, WI, July 12, 2022.

73. *Deep Learning for Molecular Biology.* Invited Short Talk, Foundations of Machine Learning and its Applications for Scientific Discovery in Physical and Biological Systems Workshop, Tysons Corner, VA, June 23, 2022.

72. *Small Molecule Generation with Property Control via Disentangled Representation Learning.* Key Speaker, AI for Bio & Medical Applications at TechConnect World Innovation Conference & Expo 2022 , June 14, 2022.

71: *Negative Broader Impacts of Large Language Models.* Invited Talk, NVTC Impact AI Summit, Responsible AI by Design: The High Road of Mission AI at Scale Panel, Tysons Corner, VA, May 11, 2022.

70. *The Journey to AlphaFold2.* AI Tea Series Talk, NSF, CISE, IIS, April 13, 2022.

69. *AI/ML-Driven Scientific Advances: A Personal Journey, Lessons, and Outlook.* Invited Speaker, IEEE Technical Talk, IEEE Washington/Northern VA Computer Society Chapter, March 15, 2022.

68. *Big Ideas and Big Data.* Invited Speaker, IEEE BigData, December 17, 2021.

67. *How to Prepare a Successful Proposal for NSF CISE/IIS.* Invited Speaker, Early CAREER Workshop, Design Automation Conference (DAC), December 05, 2021.

66. *Spatio-temporal machine learning in support of integrative biology.* Invited Speaker, AMIA Workshop on "Spatio-temporal informatics for Translational Bioinformatics", November 22, 2021.

65. *Deep Learning for Linking Chemical and Biological Space in Small Molecules and Macromolecules.* AI Track Keynote, TechConnect World Innovation Conference & Expo 2021, October 19, 2021.

64. *Computer Information, Science, and Engineering (CISE) Directorate.* Keynote, NSF Grant Conference, October 4-8, 2021.

63. *From Genotypes to Phenotypes: Calling (Deep) Modelers to Step up their Game.* Keynote, 20th Internal Workshop on Data Mining in Bioinformatics (BIOKDD), held virtually in conjunction with SIGKDD 2021, August 15, 2021.

62. *AI-Enabled Discovery of Macromolecular Structure, Dynamics, and Function.* Invited Talk, Chemical Theory Center Seminar Series, University of Minnesota, January 22, 2021.

61. *Artificial Intelligence and Data.* Invited Talk, State Department's Great Decisions, Greenspring Retirement Community, Springfield, VA, December 15, 2020.

60. *Great Disruptions and Expectations: A Perspective in Protein Modeling Research.* Keynote, 10th International Conference on Computational Advances in Bio and medical Sciences (ICCABS), December 12, 2020.

59. *Physics- and Data-driven Studies of Macromolecules.* Invited Talk, Keck Center Celebration, Rice University, October 30, 2020.

58. *A Data-driven Journey into Macromolecular Structure, Dynamics, and Function.* Invited Talk, NSF HDR Workshop on Knowledge Guided Machine Learning, August 20, 2020.

57. *An AI-aided Entry to Modeling Actuated Systems.* AI Tea Series Seminar, NSF, CISE, IIS, April 22, 2020.

46. *Discriminative and Generative Models of Protein Structure, Dynamics, and Function.* Invited Talk, Clarkson

University, Potsdam, NY, April 19, 2019.

45. *A Vision of Data-driven Discovery as the Bedrock of Convergence Research.* Invited Talk, NSF CISE/IIS, Alexandria, VA, February 06, 2019.

44. *Recurrent Neural Networks, Generative Models, and Generative Adversarial Networks.* Invited Talk, Micron Corporation, Manassas, VA, August 24, 2018.

43. *Nga Struktura, te Dinamika, dhe Funksioni i Sistemeve Molekulare dhe Inxhinerike me Algoritme Optimizimi dhe Analize Statistikore.* Invited Talk, Fakulteti i Shkencave, University of Tirana, June 29, 2018.

42. *Biomolecules in Motion: Sample-based Models of Dynamics Elucidating Function and Mechanisms in the Healthy and Diseased Cell.* Invited Talk, Symposium on Data Science and Statistics, Reston, VA, May 18, 2018.

41. *All about Energy Landscapes: Generating and Analyzing them to Predict and Characterize Protein Structure, Dynamics, and Function.* Invited Talk, Chemistry and Biochemistry Seminar, George Mason University, Fairfax, VA, April 16, 2018.

40. *From Protein Structure to Dynamics and (Dys)Function via Energy Landscapes.* Invited Talk, IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM), Kansas City, MO, November 15, 2017.

39. *From Mutations to Mechanisms and Dysfunction via Computation and Mining of Protein Energy Landscapes.* Competitively-accepted Oral Presentation, 3DSIG Satellite Meeting, Intel Mol Sys Biol (ISMB), Prague, Czech Republic, July 21, 2017.

38. *Data-driven Stochastic Optimization for Sample-based Models of Protein Energy Landscapes.* Contributed Talk, Workshop on Energy Landscapes: Structure, Dynamics and Exploration Algorithms, Telluride, CO, July 17-21, 2017.

37. *Exploration Bias in Modeling Protein Equilibrium Dynamics.* Invited Talk, University of Zurich, Zurich, Switzerland, July 12, 2017.

36. *Sample-based Models of (Altered) Protein Energy Landscapes Reveal much about (Dys)Function.* Invited Talk, Laboratory of Computational Biology Seminar Series, National Heart, Lung and Blood Institute, NIH, June 29, 2017.

35. *Of Form and Function: Stochastic Optimization Elucidates Role of Dynamics in Proteinopathies.* Invited Talk, Krasnow Institude for Advanced Study, Seminar Series , George Mason University, February 20, 2017.

34. *Sample-based Representations and Algorithms for Modeling Protein Structure and Dynamics.* Invited Talk, 6th Workshop on Logic and Systems Biology (LSB), 31st Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), July 09, 2016.

33. *Should Have Gone To Systems.* Invited Talk, Science Slam, Women@GECCO, Genet and Evol Comput Conf (GECCO), July 12, 2015.

32. *Recovering Energy Landscapes and Mapping Functionally-relevant Structural Transitions.* Highlight Talk, Computational Structural Biology Workshop (CSBW), ACM Conf on Bioinf and Comput Biol (BCB), September 20, 2014.

31. *Probabilistic Approaches to Unravel the Form to Function Relationship in Biomolecular Systems.* Seminar Series, Institute for Bioscience and Biotechnology Research (IBBR), Rockville, MD, March 10, 2014.

30. *From the Nanoscale to the Petascale: Probabilistic Algorithmic Frameworks for Characterizing Complex Biomolecular Systems in the Presence of Constraints.* Biomedical Engineering Seminar Series, University of Florida, Gainesville, FL, January 9, 2014.

29. *Advancing Biomolecular Modeling and Simulation: A Probabilistic Approach for Characterizing Complex Systems in the Presence of Constraints.* Volgenau School of Engineering Seminar, George Mason University, Fairfax, VA, October 17, 2013.

28. *Probabilistic Approaches to Protein Modeling.* Mechanical Engineering Seminar Series, Johns Hopkins University, Baltimore, MD, February 14, 2013.

27. *Genetic Programming Based Feature Generation for Automated Functional Analysis and Annotation of DNA Sequences.* Rocky Mountain Bioinformatics Conference, Aspen/Snowmass, Colorado, December 8, 2012, accepted oral presentation.

26. *Probabilistic Search Frameworks for Protein Modeling.* School of Systems Biology Seminar, George Mason University, Fairfax, VA, November 20, 2012.

25. *Of Protein Structures and Motions: Probabilistic Search and Optimization.* Applied and Computational Math Seminar, George Mason University, Fairfax, VA, November 2, 2012.

24. *Probabilistic Search Frameworks for Modeling Structures and Motions of Protein Systems.* ACM BCB Invited Talk, Orlando, FL, October 8, 2012.

23. *Stochastic Search to Map the Space of Local Minima in the Protein Energy Surface.* Fox Chase Cancer

Center, Philadelphia, PA, October 2012.

22. *Novel Perspectives on Exploring the Protein Conformational Space for Characterizing Structures and Motions in Protein Systems.* College of Information Science Seminar, Drexel University, Philadelphia, PA, October 2012.

21. *Probabilistic Methods for Structural Characterization of Protein Systems.* Computer Science Seminar, Northern Virginia Center, Virginia Tech, Falls Church, VA, March 16, 2012.

20. *Novel Algorithmic Frameworks for Protein Conformational Search.* Bioengineering Department Seminar, UMD, College Park, MD, February 10, 2012.

19. *Simplifying and Sampling the Protein Conformational Space.* Computational Materials Science Center Colloquium, George Mason University, Fairfax, VA, February 6, 2012.

18. *Probabilistic Frameworks for Protein Conformational Search: Characterization of Native Structures of Protein Chains and Protein-based Assemblies.* Rocky Mountain Bioinformatics Conf, Aspen/Snowmass, Colorado, December 10, 2011.

17. *Probabilistic Search Frameworks for Modeling Structures, Motions, and Assembly of Protein Molecules.* Computational Materials Science Center Colloquium, George Mason University, Fairfax, VA, November 28, 2011.

16. *Probabilistic Search Algorithms to Compute Conformations of the Protein Native State.* Chemistry Department Seminar, GMU, Fairfax, VA, September 29, 2011.

15. *A Probabilistic Framework for the Characterization of the Protein Native State.* Computer Science Seminar, Lehigh University, Bethlehem, PA, March 16, 2011.

14. *Combining Evolutionary Algorithms with Supervised Learning to Extract Signals from Biological Data.* BioLearn Workshop, BIONETICS, Boston, MA, December 02, 2010.

13. *Mapping Conformational Spaces of Protein Molecules.* Computer Science Seminar, University of Massachusetts at Boston, Boston, MA, December 01, 2010.

12. *Characterizing Biological Systems at the Molecular Level.* ACE Scholars Research Highlights Invited Talk, George Mason University, Fairfax, VA, October 13, 2010.

11. *Probabilistic Methods to Compute Biologically-active Protein Conformations.* Computer Science Seminar, College of William and Mary Williamsburg, VA, June 1, 2010.

10. *Computational Aspects of Sequence, Structure, and Function in Protein Molecules.* NCBI CBB Seminar, NIH, MD, Jun 18, 2009.

9. *Motions and Assembly of Biological Molecules.* ACE Scholars Program Seminar, George Mason University, VA, Mar 17, 2009.

8. *Geometric Algorithms for Biological Research: Everything is a Puzzle After All.* GRAND Seminar Series, George Mason University, VA, Oct 16, 2008.

7. *From Atoms to Molecules to Machines: Computing Protein Motions to Elucidate Function.* Bioinformatics Colloquium, George Mason University, VA, Oct 7, 2008.

6. *A Multiscale Framework for the Characterization of Protein Native States.* National Meeting of the American Chemical Society (ACS), New Orleans, LA, Apr 6, 2008.

5. *Computing Structural Flexibility in the Protein Native State.* University of Chicago, Chicago, IL, Feb 6, 2008.

4. *Characterizing Native Flexibility in Proteins.* Fox Chase Cancer Center, Philadelphia, PA, Jan 23, 2008.

3-1. These talks were during Shehu's research as a graduate student and can be found on our lab's website.

Public Engagements & In the Media

19. How AI is Transforming Higher Education, CAIO Connect, November 11, 2025.

18. Is Society Ready for Weapons that Think for Themselves, Octoboer 23, 2025. This is a Washington Post Video Story by David Bruns, featuring AI experts.

17. AI-in-Gov Inside the Black Box, AI-in-Gov Council, 2025 – present. This is a podcast I host biweekly together with my industry co-chair of the Council.

16. The New Thing on Campus: Why Universities are Appointing their First Chief AI Officers, Fortune, September 03, 2025.

15. AI goes Systemic in Higher Education, CIO.com, Feature, August 25, 2025.

14. Chief AI Officer: Higher Ed's New Leadership Role, e.Republic Center for Digital Innovation, June 23, 2025.

13. Q&A: George Mason University CAIO Directs AI Strategy, EdTech Magazine, May 07, 2025.

12. AACRAO "For the Record" Series Podcast — AI In Higher Education, March 18, 2025.

11. Podcast — Navigating AI's risks and rewards, January 21, 2025.

10. Potomac Local News, George Mason Invests in AI Future: Dr. Amarda Shehu — Potomac Local News Podcast, January 10, 2025.

9. Key Take Aways from the U.S. National Security Memorandum and Framework, Special Competitive Studies Project, Nov 27, 2024.

8. Unpacking the "AI wardrobe:" How national policies are shaping the future of AI, OECD, Oct 30, 2024.

7. LLMs in Government: Balancing Innovation and Risk. AI, Government, and the Future Podcast Series, Sep 04, 2024.

6. Mason professors are researching hacker psychology to defend against cyberattacks. The George, May 02, 2024.

5. Generative AI and Transformed Economies. Fairfax County Times, February 2024.

4. How generative AI tools like ChatGPT could revolutionize business. Dell Perspectives, March 01, 2023.

3. AI for Human Biology and Health: A Structure Prediction Miracle. With Good Reason, WAMU 88.5FM, December 05, 2022.

2. International Symposium on Digital Therapeutics. DNews, November 11, 2022.

1. Korea-US Digital Therapy Policy Symposium. Knews1, November 10, 2022.

F7. Teaching & Mentoring Record

Curriculum Development

UNIV 182 - AI for All: Understanding and Building Artificial Intelligence is a new course open to all Introduces artificial intelligence (AI) to undergraduate students across the university, regardless of major, starting in Fall 2025. No prior computational, engineering, or quantitative background is required. Students with a broad range of disciplinary backgrounds and interests are encouraged. The course offers an introduction to AI, guiding students through its foundations, applications, and societal impacts. Hands-on activities will enable students to analyze, apply, and create AI using intuitive, non-coding platforms, from neural networks to state-of-the-art language and foundation models. Through assignments, projects, role-based debates, discussions, critical analysis, students will examine AI's impact across diverse sectors such as healthcare, policy, climate, arts, more, while addressing ethical and societal implications. By the end of the course, students will gain both theoretical and practical AI literacy, empowering them to succeed in their chosen discipline and impact our digital society responsibly.

CS689 - Planning Motions of Robots and Molecules is a new graduate course I proposed as a technical elective (CS795 - Geometric Algorithms for Bioinformatics) and taught first in Fall 2009. The first offering introduced modeling and simulation of biological systems through analogies with robotic mechanisms and motion planning. After discussions with students and robotics faculty exposed the need for a graduate robot motion planning course, I redesigned the course to focus on robot motion planning and present special applications on biological molecules. The course has been approved as a regular course, CS689. I now teach CS689 every three semesters.

CS444 - Introduction to Computational Biology is a new undergraduate course I proposed as a technical elective (CS499 - Bioinformatics and Computational Biology I) and taught in Spring 2009-2011. The course was cross-listed as ECE401 and BINF401 to gage student interest in new inter-departmental bioinformatics and bioengineering programs. With these goals in mind, the course provided a broad view of classic computational problems in sequence, structure, and systems biology. The course was very well received and has been approved as a regular course, CS444. I now teach CS444 every three semester.

List of Courses Taught at Mason

CS485 Autonomous Robotics	Fall 2018, 2016, 2013
CS580 Introduction to Artificial Intelligence	Spring 2018, 2016
CS689 Planning Motions of Robots and Molecules	Spring 2018, 2016, 2014, 2012
CS583 Analysis of Algorithms I	Spring 2019, Fall 2017, 2014, Spring 2013, Fall 2010, 2008
CS483 Analysis of Algorithms I	Spring 2017, 2010
CS695 Network Science: Principles and Applications	Fall 2016
CS444 Introduction to Computational Biology	Fall 2012, Spring 2011
CS499 Bioinformatics and Computational Biology I (cross-listed as BINF401, ECE499)	Spring 2010, 2009
CS795 Geometric Algorithms for Bioinformatics	Fall 2009

*I have been consistently among the top-ranked faculty per teaching evaluations.

Directed Ph.D. Dissertations

16. Kabir A. *Foundation Models Meet Biology: Advancing Knowledge-Rich, Multi-modal AI,* George Mason University, June 2025. Committee: Shehu A (dissertation director and chair), Kosecka J, Yao Z, and Lei Y. *Now Tenure-track Assistant Professor at University of South Florida.*

15. Inan T. T. *Rethinking Optimization for Deep Learning Under the Umbrella of Evolutionary Computation,* George Mason University, June 2025. Committee: Shehu A (dissertation director and chair), Barbará D, Liu M, and Qiao W. *Now AI Engineer at 4A Consulting.*

14. Dua M. *Text Mining-Enalbed Distillation of AI Infrastructures,* George Mason University, June 2025. Committee: Shehu A (dissertation director and chair), Singh JP, Anastasapolous A, and Barbará D.

13. Rahman T. *Generative AI for Protein Modeling: Sampling Protein Conformation Space,* George Mason University, June 2023. Committee: Shehu A (dissertation director and chair), Kosecka J, Liu M, and Jiang W. *Now Teaching Assistant Professor at University of Central Florida.*

12. Alam F. F. *Deep Latent Variable Models for Learning Representations of Protein Tertiary Structures,* George Mason University, April 2023. Committee: Shehu A (dissertation director and chair), Duric Z, Anastasopolous A, and Qiao W. *Now Teaching Assistant Professor at University of Maryland College Park.*

11. Kamranfar P. *Machine Learning Enabled Health Monitoring and Diagnosis of Engineering Systems,* George Mason University, April 2023. Committee: Shehu A (dissertation director and chair), Lattanzi D, Barbara

D, and Yao S. *Now Teaching Assistant Professor at George Mason University.*

10. Kabir K. L. *Unsupervised Learning for Molecular Structure Discoveries,* George Mason University, June 2022. Committee: Shehu A (dissertation director and chair), Duric Z, Yao S, and Qiao W. *Now Teaching Assistant Professor at Stevens Institute of Technology.*

9. Zaman A. *Evolutionary Techniques for De Novo Protein Conformation Ensemble Generation,* George Mason University, July 2021. Committee: Shehu A (dissertation director and chair), De Jong KA, Brodsky A, and Qiao W. *Now Teaching Assistant Professor at George Mason University.*

8. Rajabi Z. *Machine Learning over Social Media: From Unsupervised User Behavioral Models to Emotion Recognition via Deep Learning,* George Mason University, April 2021. Committee: Shehu A (dissertation director and chair), Uzuner O, Anastasopoulos A, and Zhao L. *Now Applied Data Scientist at Adobe.*

7. Gogovi G. *Polymers and Biomolecules in Solvent: A Molecular Dynamics Study,* George Mason University, November 2020. Committee: Kinser J (committee chair), Shehu A (dissertation director), Kavak H, and Papaconstantopoulos DA. *Now Assistant Professor at University of Houston.*

6. Akhter N. *Summarization, Visualization, and Mining of Molecular Landscapes,* George Mason University, March 2020. Committee: Shehu A (dissertation director and chair), Barbará D, Qiao W, and Li F. *Now Teaching Assistant Professor at University of Buffalo.*

5. Veltri D. *A Computational and Statistical Framework for Screening Antimicrobial Peptides,* George Mason University, July 2013. Committee: Shehu A (dissertation director), Solka J (committee chair), Vaisman I, and Matthews B. *Now a Computational Genomics Specialist at NIH-NIAID.*

4. Hashmi I. *Probabilistic Approaches to Protein-protein Docking,* George Mason University, July 2013. Committee: Shehu A (dissertation director and chair), De Jong KA, Rangwala H, Barbara D, and Kabbani N. *Now a Teaching Assistant Professor in IST Department at GMU.*

3. Molloy K. *Probabilistic Algorithms for Modeling Protein Structure and Dynamic,* George Mason University, January 2015. Committee: Shehu A (dissertation director and chair), Barbara D, Blaisten-Barojas E, and Lien J-M. *Now a tenure-track Assistant Professor at James Madison University.*

2. Kamath U. *Evolutionary Machine Learning Approach for Big Data Sequence Mining,* George Mason University, December 2013. Committee: De Jong KA (dissertation director and chair), **Shehu A** (dissertation co-advisor), Domeniconi C, and Arciszewski A. *Now Chief Analytics Officer at Digital Reasoning.*

1. Olson B. *Evolving Local Minima in the Protein Energy Surface,* George Mason University, July 2013. Committee: Shehu A (dissertation director and chair), De Jong KA, Blaisten-Barojas E, Kosecka J, and Lien J-M. *Now Engineering Manager, Machine Learning at LinkedIn.*

Directed MS. Theses

8. Lu Y. *Predicting Traffic Speed Under the Impact of Maintenance Downtime with Graph Convolutional Networks,* George Mason University, February 2021. Committee: Shehu A (committee chair), Lattanzi D (thesis director), and Zoran Duric.

7. Sambare S. *Structure- and Energy-based Analysis of FGFR2 Kinase Mutations Revealing Differences in Cancer and Syndrome Mutations,* George Mason University, May 2019. Committee: Shehu A (thesis director), Seto D (committee chair), and Klimov D.

6. Morris D. *Snapshots and Springs: Analyzing and Reproducing the Motions of Molecules,* George Mason University, August 2017. Committee: Shehu A (thesis director and chair), Duric Z, and Molloy K.

5. Majul A. *Comparative Molecular Dynamic Simulations of 2 Helical AMPs Found in Snakes ATRA-1 and ATRA-2,* George Mason University, July 2015. Committee: Bishop B (committee chair), Shehu A (thesis director), and Mikell P.

4. Veltri D. *Sequence-based Classification of Antimicrobial Peptides,* George Mason University, March 2013. Committee: Shehu A (thesis director), Vaisman I (committee chair), and Bishop B.

3. Hashmi I. *A Probabilistic Search Algorithm for Protein-Protein Docking,* George Mason University, November 2012. Committee: Shehu A (thesis director and chair), De Jong K, and Lien J-M.

2. Olson B. *Probabilistic Search Algorithms for Protein Structure Prediction,* George Mason University, November 2011. Committee: Shehu A (thesis director and chair), Kosecka J, and Lien J-M.

1. Molloy K. *Variable-Length Fragment Assembly in a Probabilistic Protein Structure Prediction Framework,* George Mason University, June 2011. Committee: Shehu A (thesis director and chair), Duric Z, and Lien J-M.

Dissertation Advising (Committee Member of Non-Mentees)

36. Rehenuma Rodoshi (GMU, Computer Science, Comprehensive Exam Committee, chair: Jessica Lin), Fall 2025

35. Zhenyi Huang (GMU, Statistics, Dissertation Proposal committee, chair: Wanli Qiao), Spring 2024

34. Gaurab Pokharel (GMU, Comprehensive Exam committee, chair: Sanmay Das), Fall 2023

33. Milind Agrawal (GMU, Comprehensive Exam committee, chair: Antonios Anastasopolous), Fall 2023

32. Bahman Pedrood, (GMU, PhD Dissertation Pre-defense and Defense, committee chair: Carlotta Domeniconi) Spring 2023

31. Kourosh Teimouri Baghaei (GMU, Comprehensive Exam committee, chair: Antonios Anastasopolous) Spring 2023

30. Huayu Zhou (GMU, Comprehensive Exam committee, chair: Antonios Anastasopolous)   Spring 2023

29. Eric Scott, Computer Science, PhD Pre-defense, Committee Member (Committee Chair: Carlotta Domeniconi)   Summer 2022

28. Abhisekh Rana, Computer Science, Comprehensive Exam (Committee Chair: Zoran Duric)   Spring 2022

27. Jonathan Mbuya, Computer Science, Comprehensive Exam, Committee Chair,   Spring 2022

26. Abhisekh Rana, Computer Science, Comprehensive Exam, Committee Member (Committee Chair: Carlotta Domeniconi),   Spring 2022

25. Tasfia Mashiat, Computer Science, Comprehensive Exam Committee Chair,   Fall 2021

24. Bahman Pedrood, Computer Science, Comprehensive Exam and PhD Proposal Defense Committee Member (PhD Dissertation Director: Carlotta Domeniconi)   Spring – Summer 2021

23. Jooyeon Lee, Information Sciences and Technology, PhD Pre-defense and Defense Committee Member (PhD Dissertation Director: Ozlem Uzuner)   2021-present

22. Fatemah Husain, Information Sciences and Technology, PhD Pre-defense and Defense Committee Member (PhD Dissertation Director: Ozlem Uzuner)   2020-2021

21. Sivani Tadepali, Computer Science, Comprehensive Exam Committee Member (Committee Chair: Huzefa Rangwala)   Spring 2021

20. John Hamre, School of Systems Biology, PhD Pre-defense and Defense Committee Member (PhD Dissertation Director: Saleet Jafri)   2020-2021

19. Xiaojie Guo, Information Sciences and Technology, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Liang Zhao)   2019-2021

18. Angela Achary, Comprehensive Exam Committee Member (Committee Chair: Carlotta Domeniconi)   Fall 2020

17. Yong Yang, Comprehensive Exam Committee Member (Committee Chair: Carlotta Domeniconi)   Fall 2020

16. Li Zhang, Comprehensive Exam Committee Member (Committee Chair: Carlotta Domeniconi)   Fall 2020

15. Xavier Gitiaux, Comprehensive Exam Committee Member (Committee Chair: Jana Kosecka)   Spring 2020

14. Ahmed ElMolla, Computer Science, PhD Proposal Committee Member (PhD Dissertation Director: Sean Luke)   2019

13. Kahyun Lee, Information Sciences and Technology, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Ozlem Uzuner)   2019-2021

12. Jing Lei, Statistics, PhD Proposal Committee Member (PhD Dissertation Director: Wanli Qiao) 2018-2020

11. Joseph Graus, Computer Science, PhD Proposal Committee Member (PhD Dissertation Director: Yotam Gingold)   2018-2019

10. Achyuthan J.R., Civil, Environmental, and Infrastructure Engineering, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: David Lattanzi)   2018-2016

9. Christopher Siwy, School of Systems Biology, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Dmitri Klimov)   2017-2014

8. Gregory Helmick, CSI, PhD Proposal Committee Member (PhD Dissertation Director: Estela Blaisten-Barojas)   2017-2014

7. Evan Behar, Computer Science, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Jyh-Ming Lien)   2017-2013

6. Zhonghua Xi, Computer Science, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Jyh-Ming Lien)   2017-2015

5. Yoseph Abere, CSI, PhD Proposal and Pre-defense Committee Member (PhD Dissertation Director: Estela

Blaisten-Barojas) 2017-2015

4. Jose Colbes, Computer Science, CICESE-Mexico, PhD Proposal Committee Member (PhD Dissertation Director: Carlos Brizuela) 2015-2014

3. Yanyan Lu, Computer Science, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Jyh-Ming Lien) 2013-2012

2. Adam Cadien, SPACS, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Howard Sheng) 2015-2012

1. Nada Basit, Computer Science, PhD Proposal Committee Member (PhD Dissertation Director: Harry Wechsler) 2011

Student Advising (in research activities)

Postdoctoral Fellows

3. Pourya Hoseini (Fall 2020)

2. Tatiana Maximova (May 2018 - April 2015)

1. Emmanuel Sapin (December 2016 - January 2015)

Ph.D. Students

26. Shahana Shultana (Fall 2024–present) 2024–Spring 2025)

25. Samuel Blouir (Spring 2023–present)

24. Asher Moldwin (Spring 2023–present)

23. Shiva Ghaemi (Fall 2021–present)

22. Megan Herceg (Summer 2019–present

21. Yiyang (Alex) Lian (Fall 2018–present)

20. Weisen Zhao (Fall 20254)

19. Dhiman Goswami (Fall 2021–Spring 2023)

18. Yuanjie Lu (Fall 2021–Spring 2023)

17.-1. Ph.D. alumni: Anowarul Kabir, Toki Tahmid Inan, Manpriya Dua, Fardina Alam, Taseef Rahman, Parastoo Kamranfar, Kazi Lutful Kabir, Ahmed Bin Zaman, Gideon Gogovi, Zahra Rajabi, Nasrin Akhter, Erich O'Saben, Daniel Veltri, Irina Hashmi, Kevin Molloy, Uday Kamath, and Brian Olson.

M.S. Students

15. Ankit Kumar, CS		2024–present
14. Sree Ram GabbiReddy, CS		2023–present
13. Yuanjie Lu, CS		2019–2021
12. Sivani Tadepalli, CS		2018–2021
11. Sabiha Salma, CS		2020–2021
10. Prasanna Venkatesh Parthasarathy, CS		2019-2018
9. Suma Dixit, CS		2019-2018
8. Snehal Sambare, CS		2019-2018
7. Liban Hassan, CS		2018-2017
6. David Morris, CS		2017-2016
5. Ryan Moffatt, CS		2016-2015
4. Rudy Clausen, CS, now at Parsons		2015-2012
3. Amr Majul, School of Systems Biology, now at MITRE		2013
2. Seyed Farid Hendi, CS, now at Appian		2011
1. Christopher Miles, CS, now at Google		2010

Undergraduate Students Mentored in Research Activities

41. Sam Parsa (Computer Science) Spring 2024 - Spring 2025

40. Eman Ahmed (Computer Science) — Summer 2025
39. Richa Dhakal (Computer Science) — Fall 2024 - Spring 2025
38. Alejandro Capecchi Perez (Statistics) — Fall 2021 - present
37. Sanela Refai (BIO) — Fall 2021 - present
36. **Yinkai Wang** (CS) — Fall 2021 - present
35. Aowei Ding (CS) — Fall 2021 - present
34. Melanie Gipson, REU student from Georgia State University, — Summer 2021
33. Alex Felleson, REU student from Kenyon College, — Summer 2021
32. **Yuanqi Du** (CS) — Spring 2020 - present
31. Laura Alvarez (CS, Carlos III University of Madrid) — Spring 2019 - present
30. Carlos Guerra (CS) — Spring 2019 - present
29. Mansour Faragal (CS) — Spring 2019 - present
28. Cody Barrett (CS) — Spring 2019 - Summer 2018
27. Bakr Marou (CS) — Summer 2018
26. Michael Largent (CS, Indiana Institute of Technology) — Summer 2018
25. Connor Reguero (CS) — Fall 2017
24. Armen Hagopian (CS) — Summer 2017
23. Lu Lu, GMU (CS) — Summer 2017
22. **Xiaowen Fang**, GMU (CS) — Summer 2017
21. Erica Molinar, GMU (CS) — Spring 2017 - Fall 2016
20. Savindi Ranasinghe, GMU (CS) — Spring 2017 - Fall 2016
19. Bradley English, GMU (CSS/Neuroscience) — Spring 2017 - Fall 2016
18. Heather Hendy, GMU (CS) — Summer 2015 - Fall 2015
17. Jeffrey Horowitz, Rice University (CS) — Summer 2015
16. Mazyar Katouzian, GMU (CS) — Spring 2015 - Fall 2014
15. Songyue Huang, GMU (CS) — Spring 2015 - Fall 2014
14. Wint Hnin, CRA-W DREU student from Cornell College (CS) — Summer 2014
13. Herath Pilapitiya, GMU (CS) — Summer 2014 - Spring 2014
12. Ruxi Xiang, GMU (CS) — Spring 2015 - Fall 2013
11. Mahmoud Namazi, GMU (Math) — Spring 2015 - Fall 2013
10. **Jennifer Van**, GMU (CS) — Summer 2014 - Fall 2012
9. **Sameh Saleh**, GMU (ACS Bioinformatics) — Spring 2013 - Fall 2011
8. Bryn Reinstadler , CRAW-DREU student from Williams College (CS) — Summer 2012
7. Subeer Talapatra, UVA (Chemical Engineering) — Summer 2012
6. Talhah Zafar, GMU (CS) — Summer 2012
5. Justin Towson, GMU (Neuroscience) — Spring 2011 - Fall 2010
4. **Jack Compton**, GMU (CS) — Spring 2011 - Fall 2010
3. Beenish Jamil, GMU (ACS Bioinformatics) — Summer 2010 - Spring 2009
2. Rachael Chung, CRA-W DREU student from UNCC — Summer 2009
1. Anahita Mostaghim, ASSIP fellow from UVA. — Summer 2009

High-School Students Mentored in Research Activities

19. Sofia Jacik, Riverside High School — Spring 2023
18. Shaurya Singh, Riverside High School — Spring 2023
17. **Vedant Vajre**, Stone Bridge High School — Summer 2021
16. Hailena Bian, Thomas Jefferson High School — Summer-Fall 2021
15. Spencer Huang, BASIS Independent McLean — Spring-Fall 2021
14. Alan Zhang, Thomas Jefferson High School — Fall 2020 - Spring 2021

13. Demian Yutin, Thomas Jefferson High School	Spring 2019 - Fall 2018
12. Fiona Carcani, Thomas Jefferson High School	Spring 2018 - Summer 2017
11. Noah Prinzbach, West Potomac High School	Summer 2017
10. **Sharmila Roy**, Thomas Jefferson High School	Summer 2018 - Summer 2017
9. Kevin Zou, Thomas Jefferson High School	Spring 2018 - Summer 2017
8. Rishin Pandit, Thomas Jefferson High School	Summer 2017
7. Neha Damaraju, Thomas Jefferson High School	Summer 2017
6. **Rohan Pandit**, Thomas Jefferson High School	Spring 2016 - Summer 2014
5. Pranay Singh, Thomas Jefferson High School	Summer 2014, 2012
4. Scott Jordan, ASSIP fellow, W. T. Woodson High School	Summer 2012
3. Niraja Bohidar, Thomas Jefferson High School	Summer-Fall 2012
2. Nakkul Sreenivas, Chantilly High School	2012-2011
1. Subeer Talapatra, Thomas Jefferson High School	Summer 2010

Selected Student Awards (grouped by student)

26. Fardina Fathmiul Alam (Ph.D. student), Outstanding PhD Dissertation Award, Computer Science — 2023

25. Ahmed Bin Zaman (Ph.D. student), Computer Science Distinguished Academic Achievement Award — 2021

24. Nasrin Akhter (Ph.D. student)
Department of Computer Science Outstanding Graduate Student Award — May 2019

23. Kazi Lutful Kabir (Ph.D. student)
Best Paper Award, BICOB — May 2019

22. Sharmila Roychoudhoury (TJ high-school student)
Honorable Mention Poster at ACM BCB — August 2018

21. Tatiana Maximova (CS postdoctoral fellow)
Outstanding research presentation at ISMB 3DSIG — July 2016

20. Bradley English (CSS/Neuroscience undergrad)
OSCAR undergraduate apprenticeship — Fall 2016

19. Heather Hendy (CS undergrad)
OSCAR undergraduate apprenticeship — Spring 2016

18. Mazyar Katouzian (CS undergrad, graduated May 2015)
OSCAR undergraduate apprenticeship — Spring 2015

17. Songyue Huang (CS undergrad, graduates May 2016)
OSCAR undergraduate apprenticeship — Spring 2015

16. Daniel Veltri (School of Systems Biology Ph.D., graduated 2015)
Best student paper at IEEE BIBM in first-author capacity — November 2014
Travel Award, ICCABS — June 2013
Outstanding Oral Presentation, School of Systems Biology Student Research Day, Daniel Veltri — May 2013

15. Irina Hashmi (CS Ph.D., graduated 2015)
Best Poster Award, IEEE BIBM — October 2012
Travel Awards, IEEE BIBM, CRA-W Grad Cohort Workshop — May 2011
Research Assistant Fellowship — 2010 - 2011

14. Rudy Clausen (M.S. Ph.D., graduated 2015)
Guest (Intern) Researcher in the Cancer and Inflammation Program at the National Cancer Institute 2013-2014

13. Jennifer M. Van (CS undegrad, graduated 2015)
Dean's Award in Physical Sciences at the College of Science Undergraduate Research Symposium — 2014
Oustanding Project Award at the Volgenau School of Engineering Undergraduate Research Celebration — 2014
Second author of a journal paper — 2014
Second author of a refereed conference paper — 2013
Princeton MOL/QCB Summer Program — May 2013
CRA-W DREU (Distributed Research Experiences for Undergraduates) — May 2013
University of Wisconsin Madison REU — May 2013
OSCAR undergraduate apprenticeship — Spring 2013

12. Kevin Molloy (CS Ph.D., graduated 2015)
    Outstanding CS Graduate Student Award   April 2015
    Finalist for best paper award at BiCoB   March 2014
    Travel Award, ICCABS   June 2013
    Outstanding Academic Achievement Award   August 2011
    Dean Fellowship   Fall 2011 - Spring 2012
    Best Paper award at BIONETICS in second-author capacity   December 2010

11. Uday Kamath (IT Ph.D., co-advised with K. De Jong, graduated 2014)
    Honorable Mention, Humies Competition Award at GECCO   June 2012

10. Herath Pilapitiya (CS undegrad, graduated 2014)
    OSCAR undergraduate apprenticeship   Summer Intensive 2014

9. Brian Olson (CS Ph.D., graduated 2013)
   Mason VSE Outstanding Graduate Student Award   April 2013
   Outstanding Academic Achievement Award   May 2012
   Best Paper Award at BIONETICS in first-author capacity   December, 2010

8. Sameh Saleh (CS undergrad, graduated May 2013)
   First author of a refereed journal and a refereed workshop paper   2013-2012
   Second author of a refereed journal paper   2013
   Author of numerous abstracts and extended abstracts   2013-2012
   Finalist, Male, CRA Outstanding Undergraduate Researcher Award   May 2013
   Mason OSCAR Outstanding Undergraduate Research Award   May 2013
   Selected undergraduate presenter, NCUR   May 2013
   Keynote undergraduate speaker at COS Undergraduate Research Colloquium   May 2012
   OSCAR undergraduate apprenticeship   Fall 2011

7. Bryn Reinstadler (CS Williams College, graduated 2014)
   CRA-W DREU (Distributed Research Experiences for Undergraduates) in Shehu Lab May 2012

6. Scott Jordan (Woodson high school, now at RIT)
   ASSIP high-school fellowship   June 2012

5. Justin Towson (CS undergraduate, graduated 2012)
   OSCAR undergraduate apprenticeship   Fall 2010

4. Jack Compton (CS Ph.D., graduated 2011)
   Second author of a refereed journal paper   2012

3. Beenish Jamil (CS undergraduate, graduated 2011)
   Honorable Mention, CRA Outstanding Undergraduate Research Award   May 2011
   CRA-W DREU (Distributed Research Experiences for Undergraduates)   May 2011

2. Rachael Chung (CS undergradute, UNCC, now CS Ph.D.)
   CRA-W DREU (Distributed Research Experiences for Undergraduates) in Shehu Lab May 2009

1. Anahita Mostaghim
   ASSIP undergraduate fellowship   June 2009

F8. Professional Service

National Leadership

Taskforces

National Academies of Sciences, Engineering, and Medicine Working Group on Biosecurity, member, 2024-2025. Report published here.

Taskforce on 'Generative AI Risks and Associated Controls' in NIST AISIC Risk Management Working Group, member, 2024.

Taskforce on 'Case Studies, Best practices, Piloting, and Reference Implementations of a GAI profile of the NIST AI RMF (NIST AI 100-1)' in NIST AISIC Risk Management Working Group, member, 2024.

State Council of Higher Education for Virginia EO30 Taskforce.

Advisory Boards

Member of the U.S. Department of Energy Joint Genome Institute's Advisory Committee (JAC), September 2025 – present.

Founding Member of the Center for Digital Education's Higher Education AI Council, August 2025 – present.

Member of the Advisory Board of the University of Virginia, Department of Electrical and Computer Engineering, January 2024 – present.

Member of the Advisory Board of the Commonwealth Science & Technology Ethics Policy (STEP) Collaborative, 2024 – present.

Member of the External Advisory Board of the NSF Center for Computer Assisted Synthesis (C-CAS), 2024 – present.

Scientific Societies

Member, ACM's US Technology Policy Committee and Chair of AI & Algorithms, Digital Governance Sub-Committee, 2024 – present.

Editorial Leadership

Editorial Positions

Guest Editor of International Journal of Molecular Sciences (IJMS, IF: 6.208) Special Issue on Deep Learning for Modeling the Structure, Dynamics, and Function of Small and Large Molecules, 2022-2023.

Guest Lead Editor of International Journal of Molecular Sciences (IJMS, IF: 6.208) Special Issue on Recent Advances in Computational Structural Bioinformatics, 2022-2023.

Co-editor of Section on Theory and Simulation/Computational Methods in the Current Opinion in Structural Biology Journal, 2019-2021.

Associate Editor of IEEE/ACM Trans Comput Biol & Bioinf Journal, April 2017-present.

Guest Editor of Biomolecules, 2019-2018, special issue.

Guest Co-editor of IEEE/ACM Trans Comput Biol & Bioinf Journal, 2017-2018 (special issue of ACM-BCB 2017)

Guest co-editor, J Biomedical and Health Informatics 2017-2018 (special issue of ACM-BCB 2017).

Guest Editor of PLoS Comput Biol, May 2017.

Editorial board member, Intl J. of Data Mining and Bioinformatics (IJDMb), 2012-2017.

Guest Co-editor of special collection on Macromolecular Structure and Dynamics of PLoS Comput Biol 2015.

Co-editor of Robotica 2015 (special issue).

Co-editor of IEEE/ACM Trans Comput Biol and Bioinf 2015 (special issue).

Co-editor of J Comput Biol 2015 (special issue).

Guest associate editor of Education Collection of PLoS Comput Biol 2014.

Co-editor of BMC Struct Biol 2013 (special issue).

Co-editor of J Bioinf and Comp Biol 2012 (special issue).

Co-editor of J Bioinf and Comp Biol 2011 (special issue).

Conference and Workshop Leadership

Conference and Conucil Chairships

Organizer, AI-in-Gov Council Signature Event: Converge AI Forum, September 18, 2025, Arlington VA.

Senior Program Committee Member of AAAI 2026, Singapore.

Co-Organizer, VASEM Annual Summit Virginia AI: Charting the Future of Virginia Summit, 2025.

Chair of ACM/IEEE Trans Bioinf and Comp Biol (TCBB) Steering Committee, ACM representative, 2018-2022

Session Chair of AI for Biomedical Applications Track, Tech Connect World Innovation and Expo 2021, National Harbor, MD.

Senior Program Committee Member of KDD 2020, San Diego, CA.

Tutorial chair of ISMCO 2019, Lake Tahoe, NV.

General chair of ACM BCB 2018, Washington, D.C.

Program co-chair of ACM BCB 2017, Boston, MA.

"Undergraduate research highlights" section writer of ACM SIBIO newsletter, 2017.

Program co-chair of IEEE BIBM 2015, Washington, D. C.

Tutorials co-chair of ACM BCB 2014, Newport Beach, CA.

"Computer Scientist in Profile" section writer of ACM SIGBIO newsletter, 2012-2014.

Local arrangement chair of ACM BCB, Washington, D.C, September 22-25, 2013.

Chair of Systems Biology session, ACM BCB, October 9, 2012.

Co-chair of Poster Session at IEEE BIBM, October 4-7, 2012.

Organizing Committee vice-chair of BIONETICS, Dec. 1-3, 2010.

Co-organizer of Bioinformatics track of BIONETICS, Dec. 1-3, 2010.

Organization of Workshops and Tutorials

"FMs4Bio" Workshop at AAAI 2025, Philadelphia, PA.

"LLMs4Bio" Workshop at AAAI 2024, Vancouver, Canada.

"Ethics and AI Undergraduate Minor at George Mason University: Planning Workshop" at George Mason University, March 25, 2022. (with Jesse Kirkpatrick/Philosophy, Alexander Monea/English, Rachel Jones/Philosophy, and Peng Warweg/CAHMP).

"Spatial & Spatial-Temporal informatics: Methods, Tools and Emerging Opportunities for Translational Bioinformatics" Workshop (W23) at AMIA 2021 Annual Symposium, October 31, 2021, San Diego, CA. (with Arvind Rao/U Michigan Ann Arbor, Mary Saltz/Stony Brook, Shashi Shekhar/U Minnesota, Joel Saltz/Stony Brook Medicine, and Li Zhu/NIH).

"Modeling Macromolecular Structures and Motions: Computational Methods for Sampling and Analysis of Energy Landscapes" Tutorial at ACM BCB 2018, Washington, DC.

"Computational Structural Biology Workshop" at ACM BCB, August 20, 2017, Boston, MA.

"Women@GECCO" Workshop at GECCO, July 15, 2017, Berlin, Germany.

"Evolutionary Computation in Computational Biology" Workshop at GECCO, July 16, 2017, Berlin, Germany.

"Robotics-inspired Algorithms for Modeling Protein Structures and Motions" Tutorial at ACM BCB 2017, Boston, MA.

"Women@GECCO" Workshop at GECCO, July 2016, Denver, Colorado.

"Evolutionary Computation in Computational Biology" Workshop at GECCO, July 2016, Denver, Colorado.

"Evolutionary Algorithms for Protein Structure Modeling" Tutorial at ACM BCB, October 2016, Seattle, Washington.

"Computational Structural Biology Workshop" at IEEE BIBM, November 11, 2015, Washington, D.C.

"Evolutionary Computation in Computational Biology" Workshop at GECCO, July 11, 2015, Madrid, Spain.

"Evolutionary Algorithms for Protein Structure Modeling" Tutorial at GECCO, July 11, 2015, Madrid, Spain.

"Computational Structural Biology Workshop" at ACM BCB, September 20, 2014, Newport Beach, LA.

"Robot Motion Planning Methods for Modeling Structures and Motions of Biomolecules" Tutorial at ACM BCB, September 20, 2014, Newport Beach, CA.

"Evolutionary Search Algorithms for Protein Modeling: From De-novo Structure Prediction to Comprehensive Maps of Functionally-relevant Structures of Protein Chains and Assemblies" Tutorial at GECCO, July 12, 2014, Vancouver, Canada.

"NSF CISE CAREER Writing Workshop" March 31, 2013, Arlington, VA.

"Artificial Intelligence and Robotics Methods in Computational Biology" Workshop at AAAI, July 14, 2013 Bellevue, WA.

"Computational Structural Biology Workshop" at ACM BCB, September 22, 2013, Washington, D.C.

"From Robot Motion Planning to Modeling Structures and Motions of Biological Molecules" Tutorial at ACM BCB, September 22, 2013, Washington, D.C.

"Computational Structural Biology Workshop" at IEEE BIBM, October 4, 2012, Philadelphia, PA.

"Computational Structural Biology Workshop" at IEEE BIBM, November 12, 2011, Atlanta, GA.

"Evolutionary Computation and Machine Learning in Bioinformatics Workshop" (BioLearn) at BIONETICS, Dec. 1-3, 2010, Boston, MA.

Referee Activities

Grant proposal referee for Netherlands Organization for Scientific Research; Multidisciplinary University Research Initiative, Army Research Office; Spark Initiative, Swiss National Science Foundation; Advanced Research Projects Agency - Energy (ARPA-E); National Defense Science and Engineering Graduate Fellowships; NSF panels CISE-IIS, CISE-FET, CISE-CCF, CISE-CSSI, CISE-SI2, BIO-MCB; NIH study sections NINDS NST-2 (K99/R00 and F32); ZRG1 Special Emphasis S10 (study section chair); BST-80 AREA (R15) Bioengineering; BDMA, Special Emphasis Panel (SEP) for Biomedical Research Shared Instrumentation (S10); Bioinformatics - Topics in Computational Biosciences Special Emphasis Shared and High-End Instrumentation; Accelerating Scientific Discovery (ASDI) (Netherlands e-Science Center + Netherlands Organisation for Scientific Research); AgreenSkills (EU + INRIA).

Journal paper referee for Nature Methods, Nature Communications, FEBS Letters, Bioinformatics, PLoS Comput Biol, PLoS One, J Phys Chem Lett, Scientific Reports, F1000 Research, BMC Genomics, Proteins: Struct, Funct, and Bioinf, Proc Natl Acad Sci (PNAS), J Amer Chem Soc (JACS), Biophysical J, Biochimica et Biophysica Acta (General Subjects) Structural Dynamics, J of Artificial Intelligence Research (JAIR), Neural Processing Letters (NEPL), Robotics and Automation Letters (RA-L), IEEE Transactions on Robotics (T-RO), Robotica, IEEE Trans Evol Comput (TEVC), J of Applied Mathematics and Computation, Entropy J, IEEE Trans on Comp Biol and Bioinf (TCBB), IEEE Transactions on NanoBioscience, BMC Structural Biology J, Molecules, J Computer-aided Molecular Design, Proteome Science J, Evolutionary Bioinformatics, Computational Biology and Chemistry J, Intl J Mol Sciences, Computers in Biology and Medicine, Computational and Mathematical Methods in Medicine, J Chem Info and Model, J Comput Chemistry, Molecular Biology Reports, and more.

Conference paper referee for AAAI, NeurIPS, ACM Bioinformatics and Computational Biology Conference (ACM BCB), IEEE Bioinformatics and Biomedicine (BIBM), Intl Conf Res Comp Mol Biol(RECOMB), Intelligent Systems Mol Biol (ISMB), Intl Conf on Bioinf and Comput Biol (BiCoB), Symposium on Computational Geometry (SoCG), Comput Struct Biol Workshop (CSBW), Intl Conf Comp Sys Bioinf (CSB), Intl Workshop Algo Found of Robotics (WAFR), IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS) Inlt Conf Bio-inspired Models of Network, Info, and Comput (Bionetics) IEEE Intl Conf Net Dig Tech (NDT)

Professional Associations

American Association for Advancement of Science (AAS)

IEEE, ACM

American Institute for Medical and Biological Engineering (AIMBE)

International Society for Computational Biology (ICSB)

Biophysical Society

Protein Society

American Chemical Society (ACS)

National Council on Undergraduate Research (NCUR)

Other Scientific Outreach

Panelist, "What it Takes to Lead in the AI Era," The Chronicle of Higher Education, December 04, 2025, Webinar.

Panelist, "BLS Board Meeting Event: Enabling Scientific insights in the Life Sciences and Biotechnology through AI," National Academies of Science, Engineering, and Medicine, October 30, 2025, Washington, DC.

Panelist, Session One: AI Fundamentals for Humanists, "AI and the Humanities" Workshop, co-organized by the Center for Humanities Research (Alok Yadav) and the College of Engineering and Computing (Amarda Shehu), October 07, 2025, Fairfax, VA.

Panelist, "AI in Military Housing" at the Military Housing Association Conference, August 13, 2025, Arlington, VA.

Panelist, "AI and Biotechnology" at Artificial Intelligence and Global Risk Media Briefing, Federation of American Scientists, April 11, 2025, Washington, D.C.

Panelist, "Finding Common Ground: Dismantling Division Through Research" at Mason Graduate Interdisciplinary Conference Panel, April 04, 2025, Fairfax, VA.

Steering Committee member, Impact AI Symposium, Northern Virginia Technology Council, 2025-2024.

Panelist, "Role of AI in Fairfax County Public Schools" at Fairfax County Federation of Citizen's Associations, March 25, 2025, Falls Church, VA.

Panelist, "AI Applications and Ethical Considerations" at ECEDHA, March 23, 2025, Norfolk, VA.

Panelist, "AI at George Mason University" at Women in Tech and Women of Color in STEM, March 17, 2025, Fairfax, VA.

Panelist, Association of Public and Land-grant Universities (APLU) Summer Communications Summit, June 24, 2024, Fairfax, VA.

Panelist, AI Roundtable Discussion, CCI, March 28, 2024, Arlington, VA. Outcome of panel: 2024: Cybersecurity for AI and AI for Cybersecurity.

Panelist, Roundtable Discussion on Standards in the Executive Order in Artificial Intelligence, Center for Strategic and International Studies, January 30, 2024, Washington D.C.

Panelist, "AI Applications: Biological Systems", Foundations of Machine Learning and its Applications for Scientific Discovery in Physical and Biological Systems Workshop, June 23, 2022, Tysons Corner, VA.

Panelist, "Responsible AI", NVTC Impact AI, May 11, 2022, Tysons Corner, VA.

Judge, Student AI Research Proposals, Ideaventions Academy for Mathematics and Science, December 17, 2020, Reston, VA.

Panelist, "Future of the Architectural Profession as it Related to Data Science, Machine Learning, and AI", AIA Leadership Series, D.C. Local Chapter, 2019, Arlington, VA.

Panelist, "Ready or Not, Artificial Intelligence and Machine Learning Arrive", Government IT Sales Summit 2018, Reston, VA.

ISCB Youth Bioinformatics Conference (YBS), panelist, George Mason University, January 12, 2019.

"Undergraduate research highlights" section contributor of ACM SIGBio newsletter, 2017.

Judge in Computer Science Category of the (international) Undergraduate Awards, 2017-2015

Executive Supporter of Girls Computing League, 2016-2015.

Women in Bioinformatics Panel Member at ACM BCB, 2014.

George Mason University NSF CAREER panelist, May 20, 2014.

State Department 3rd Young Scientist Forum, People to People Exchange, September 18, 2012.

George Mason University NSF CAREER panelist, April 18, 2012.

Women in Bioinformatics Panel Member at ACM BCB, 2012.

Organizer of Chantilly High School Bioengineering Tour, June 17, 2011.

Co-organizer of High School Bioengineering Summer Internship Program, Summer 2011.

Two-body Problem Panel Member at Grace Hopper Conference, October 2009.

F9. National and Institutional Leadership

NSF Highlighted Activities   **What is shown here has been declassified and is shared with permission.**

Leader, NSF-wide Working Group on Data Science Education and Training Program (2021–2022). Led the full conceptualization-to-clearance process for a new cross-directorate program.

Leader, CISE–EHR Working Group on K–12 Data Science Training Program (2021–2022). Led all stages of the conceptualization and clearance of a new Dear Colleague Letter.

Leader, NSF-wide Working Group on HDR: Data Science Corps (2019–2021). Directed the revision-to-clearance process for the 2021 HDR:DSC competition, coordinated internal timelines and panel assignments, developed award recommendations and budget plans, oversaw portfolio analysis and reporting to NSF leadership, and worked with NSF Communications to highlight program outcomes in NSF News and blogs.

Member, NSF-wide Working Group on Molecular Foundations for Biotechnology; CISE Lead (2021–2022). Led CISE-side conceptualization and solicitation revision, ensuring AI was a central methodological component of the program.

CISE Liaison Program Director for NSF–Czech Science Foundation (GACR) collaboration (2019–2021). Adjudicated requests and coordinated CISE participation in the bilateral program.

Member, CISE–IIS Working Group on AI-Enabled Discovery (2020–2022). Helped organize initiatives at the AI–science interface, including leading a \$1B AI-Enabled Discovery "Big Idea" pitch to CISE leadership and the AD.

NSF representative to the Big Data Interagency Working Group (2019–2021), coordinating with other federal agencies on large-scale data initiatives.

Member, NSF–NIH Collaboration Working Group (2019–2021), conceptualizing joint opportunities and cross-agency research programs at the intersection of computing, data, and biomedicine.

CISE Coordinator for NSF Coronavirus RAPID (2020). Adjudicated RAPID requests, identified appropriate programs, coordinated interest-to-award processes, tracked awards, and reported data and portfolio trends to CISE and NSF leadership.

Conceptualized and catalyzed a two-day NSF-funded symposium on novel COVID-19 therapeutics, led by Jure Leskovec (Stanford) and Marinka Zitnik (Harvard). Assisted with recruitment of a diverse set of speakers and broad advertising. The symposium attracted 1,840 participants from academia, industry, and non-profits and led to prominent interdisciplinary research on SARS-CoV-2 proteomics and repurposed and novel therapeutics.

Member, NSF-wide Traveling Working Group in AI & Nanobiology, NSF Multiplier Mission for the Czech Republic (2019–2020). Evaluated in-country capabilities in AI and nanobiology and, together with PDs from EHR and MPS, supported OISE in conceptualizing and clearing the NSF–GACR initiative that went into effect in 2021.

VP and Chief AI Officer Highlighted Activities

Formulating and executing the AI² Nexus, which positions Mason as a nexus for AI innovation around four principles: integrating AI into education, research, and operations; inspiring the future workforce through AI; innovating in responsible AI-enabled discovery across disciplines; and impacting society through partnerships and community engagement.

Leading an AI Visioning Taskforce (70+ faculty, staff, and students) across all academic and non-academic units and campuses (including Mason Korea) to develop a shared AI strategy under a strong shared-governance model. This work exemplifies collaborative, decisive leadership that engages, supports, and empowers diverse stakeholders.

Serving as a leader, mediator, and implementer for strategic AI initiatives that advance the university's research and academic mission. I work closely with partners such as Microsoft and Cloudforce to cultivate relationships, secure funding, and coordinate collaborative strategies, while regularly engaging with the President, Provost, Deans, and Associate Deans to align AI priorities with Mason's broader institutional vision.

In close collaboration with the CIO, securing a partnership with Microsoft and Cloudforce to launch PatriotAI, an academic platform providing access to over 1,800 generative AI models for faculty, students, and staff. Under my leadership, the AI Taskforce rapidly articulated and published principles and guidelines for safe use of AI at

Mason, the first such guidance in Virginia, as an early instantiation of the Integrate AI initiative.

Co-leading the Inspire with AI initiative to bring AI literacy to all faculty, students, and staff. This includes a scaffolded approach through the learning management platform, the design and launch of AI4ALL (Fall 2025) to open AI to all undergraduates, integration of AI across curricula, and creation of new cross-college programs that advance key societal themes.

Through the Innovate AI and Impact with AI pillars, driving expansion of Mason's research enterprise via strategic investments and interdisciplinary collaboration. This includes establishing and strengthening centers, securing competitive funding, and forging partnerships with industry, government, and philanthropy. I work with faculty to support ambitious research agendas, help junior colleagues build strong trajectories, and align research efforts with workforce needs and societal challenges so that Mason's AI, computing, and science research translates into lasting real-world impact.

AVPR Highlighted Activities

As AVPR, I was responsible for Fuse programming and activation, a first-in-the-region public–private-partnership (P3) building central to Mason's re-envisioning of the Arlington Campus as Mason Square. I remain actively involved with Fuse as a member of its governing board.

To better connect innovation with impact, I conceptualized and implemented the IDIA P3 Faculty Fellowship Program, a competitive award program providing research support to Mason faculty. The program helped build IDIA's identity and community, expanded Mason's public–private partnership portfolio, and more closely aligned Mason's R&D with local, regional, and national industry.

I also created the IDIA Predoctoral Fellowship Program, a competitive initiative that provides full support to predoctoral students across Mason and treats PhD students as agents of change tackling interdisciplinary "wicked" problems. The program established a predoctoral cohort model and gives students agency to define emerging research problems and assemble cross-disciplinary faculty teams with the required expertise.

I institutionalized relationships with industry and government through the IDIA CONNECT Series, a series I designed to bring leaders from industry, federal and local government, funding agencies, and non-profits together with Mason faculty, researchers, and students around areas of mutual interest. Among its outcomes, the series has significantly grown strategic public–private partnerships.

To further champion interdisciplinary research and education, I launched the IDIA AI Innovation Symposium, an interdisciplinary symposium that convenes faculty and researchers around organically emerging AI-centric themes. The symposium has been followed by numerous thematic convenings, some strategically linking units such as the College of Engineering and Computing with the College of Humanities and Social Sciences around language technologies, and others focused on AI, policy, society, and education.

AD-CEC Highlighted Activities

Led the full process—from ideation to record-time SCHEV approval—for Virginia's first Master's in AI. Working closely with industry partners, I translated workforce needs into program learning outcomes and collaborated with faculty to shape the curriculum. Launched in Fall 2025, this degree is the first major milestone of the College's AI Roadmap, which I initiated as Associate Dean for AI Innovation and continue to advance at both the College and University levels.

As Associate Dean for Research, I am leading a data-informed strategy to strengthen and future-proof the College's research enterprise. This includes strategic investment in interdisciplinary centers and signature research themes; building high-impact, visionary research teams; cultivating industry partnerships through centers and councils; driving strategic fundraising initiatives; and spearheading curricular innovations that deliver a competitive and distinctive student experience.

Spearheaded the creation of M-CAI^{2}S (Mason Center for AI Innovation for Society), a joint center bridging the College of Engineering and Computing with the Schar School of Policy and Government to advance interdisciplinary AI research and policy engagement. Played a key role in launching ISEAI (Infrastructure Security in the Age of AI), positioning it toward Industry–University Cooperative Research Center designation. Founded and championed the AI-in-Gov Council in January 2025, a public–private partnership bringing together government CXOs, public-sector technology providers, and faculty to catalyze research aligned with regional and national needs. These efforts demonstrate my ability to cultivate strategic partnerships and position institutions at the intersection of computing, policy, and societal impact.