Stephen Szwiec

RESEARCH COMPUTING SPECIALIST · PHD STUDENT

Fargo, ND

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Personal Profile

Currently advancing doctoral research in multi-scale modeling of stochastic polymer systems at NDSU Materials and Nanotechnology program while serving as Scientific Software Specialist at the CCAST high-performance computer, delivering critical computational infrastructure for cutting-edge scientific discovery.

Education

North Dakota State University
Fargo, ND

PhD. Materials and Nanotechnology
01.2022 – Present

- **Studies:** Condensed Matter Physics, Quantum Mechanics, Materials Chemistry, Nanotechnology, Computational Methods
- **Advisor:** Dr. Bakhtiyor Rasulev
- **Research:** Developing predictive models and computational methods for advanced materials, specializing in QSPR modeling of photovoltaic polymers, molecular dynamics simulations for biofouling, and novel computational tool creation.

Minot State University
Minot, ND

B.Sc. in Bioinformatics and Computational Biology, Mathematics Minor
01.2019 – 12.2021

- **Studies:** Genetics and Molecular Biology, Cybersecurity, Database Management, Statistical Models, Unix Environment
- **Research:** Genome-wide association studies of complex traits in field pea, chickpea, and lentil
  Cybersecurity risk model for IoT in US crop agriculture

Work Experience

Scientific Software Specialist
Fargo, ND

NDSU – Center for Computationally Assisted Science and Technology
11.2023 – Present

- Architected and optimized high performance computating workflows across scientific domains.
- Managed comprehensive software stack deployment, automating installation and configuration of sicnetific software.
- Colaborated directly with researchers to identify and implement software solutions, including over 150 ticket resolutions in 2024.
- Created technical curriculum materials for training and onboarding new users to HPC resources, and delivered training sessions.
- Provided specialized technical consulting for NSF-funded research projects requiring advanced computational resources.

Graduate Research Assistant
Fargo, ND

NDSU – Department of Coatings and Polymeric Materials
01.2022 – Present

- Researched photovoltaic polymer materials using Quantitative Structure-Property Relationship (QSPR) machine learning methods.
- Developed combinatorial descriptor generation and machine learning software.
- Engineered multi-scale molecular dynamics simulations and free energy modeling for biofouling removal applications.
- Created molecular docking pipelines for toxicity prediction with automated analysis workflows.
- Administered laboratory computational infrastructure including workstation cluster management and software deployment.
- Mentored undergraduate researchers in computational methods and scientific programming practices.

Research Computing Intern
Fargo, ND

NDSU – Center for Computationally Assisted Science and Technology
05.2023 – 11.2023

- Authored technical documentation for HPC software deployment and containerization best practices.
- Optimized scientific application builds with architecture-specific tuning.
- Provided technical support to researchers using HPC resources.
- Assisted in the development of training materials for HPC users.

Undergraduate Research Assistant
Minot, ND

NDSU – Department of Plant Sciences
05.2020 – 12.2021

- Engineered compute infrastructure for deploying genomics pipeline integrating Tassel5, VCFtools, and ADMIXTURE.
- Developed high-throughput GWAS pipeline, using R and targeting high-performance computing resources.
- Maintained and audited legacy SQL database systems for phenotypic data management and retrieval.
- Redesigned inventory management system, reducing experimental setup time by a factor of four, and enhancing ergonomics.
- Standardized nomenclature system for pulse plant experimental trials, enhancing data collection consistency.

Computer Science Tutor
Minot State University

Minot, ND

08.2021 – 12.2021

- Tutored students on computer programming, data structures, algorithms, and Unix environment.
- Generated didactic materials supplementing student coursework.

Computer Lab Systems Administrator
Minot State University

Minot, ND

01.2021 – 12.2021

- Refurbished PCs for computer science and mathematics department labs.
- Coordinated with university information technology staff to deploy needed operating systems and software.
- Ensured systems met technical requirements for professors.

Undergraduate Research Assistant
New Mexico Institute of Mining and Technology

Socorro, NM

05.2021 – 07.2021

- Created economic risk data model simulating cybersecurity risk exposure to US precision agriculture using publicly available USDA datasets.
- Presented findings during REU cybersecurity symposium.

Chemistry Lab Assistant
Minot State University

Minot, ND

10.2019 – 04.2020

- Performed day-to-day tasks for chemistry laboratory and campus stockroom.
- Performed inventory management of chemicals and equipment.
- Assisted university faculty in preparation of laboratory experiments.

Note Preparer
Minot State University

Minot, ND

01.2019 – 12.2019

- Took notes for students with disabilities in computer science and chemistry courses.
- Upheld standards for both HIPAA Privacy Rule and Rehabilitation Act of 1973 for information security.

Publications

QSPR Modeling of the Power Conversion Efficiency of Fullerene Derivatives as electron acceptors in P3HT-based organic solar cells
Stephen Szwiec, Bakhtiyor Rasulev, Gerardo Casañola-Martin

Fargo, ND

(in progress)

- Curated data and developed predictive models for the power conversion efficiency of fullerene derivatives in organic solar cells.
- Authored and edited manuscript, and performed data analysis.

Predictive Toxicity Modeling and Virtual Library Design of Fullerene Derivatives: Insights from Quantitative Structure-Activity Relationship Analysis
Amirreza Daghighi, Madeline Williams, Stephen Szwiec, Gerardo Casañola-Martin, Bakhtiyor Rasulev

Fargo, ND

(in preparation)

- Machine learning and computational modeling of fullerene derivative toxicity.
- Edited manuscript and provided computational support.

In Silico Prediction of the Biodegradability of Chlorinated Compounds: Application of Super Learner QSBR Approach
Meade Erickson, Denys Vasyutyn, Marvellous Ngongang, Amirreza Daghighi, Stephen Szwiec, Gerardo Casañola-Martin, Bakhtiyor Rasulev

Fargo, ND

(pre-print)

- Machine learning and computational modeling of chlorinated polymer biodegradability.
- Introduction and background of the project; performed programming and data analysis.
- doi:10.26434/chemrxiv-2024-p7dx4

CombinatorxPy: Advancing Mixture Descriptors for Computational Chemistry *Fargo, ND*

Rahil Ashtari Mahini, Gerardo Casañola-Martin, Stephen Szwiec, Simone Ludwig, Bakhtiyor Rasulev

02.2025

- Python package implementing novel method to derive numerical representation of chemical mixtures based on a combinatorial approach.
- Conceptualition and methodology of software, review, and editing of manuscript.
- permalink: https://github.com/ElsevierSoftwareX/SOFTX-D-24-00534

Integrated machine learning, computational, and experimental investigation of compatibility in oil-modified silicone elastomer coatings *Fargo, ND*

Anas Karuth, Stephen Szwiec, Gerardo Casañola-Martin, Achiya Khanam, Maryam Safaripour, David Boucher, Wenjie Xia, Dean C. Webster, Bakhtiyor Rasulev

09.2024

- Modeling framework that integrates machine learning (ML), statistical thermodynamics, molecular dynamics simulation, and surface characterization techniques to describe a bio-release coating.
- Authored, edited manuscript, and performed data analysis.
- doi:10.1016/j.porgcoat.2024.108526

Harnessing Genetic Diversity in the USDA Pea Germplasm Collection Through Genomic Prediction *Fargo, ND*

Md. Bari, Peng Zheng, Indalecio Viera, Hannah Worral, Stephen Szwiec, Yu Ma, Dorrie Main, Clarice J. Coyne, Rebecca McGee, and Nonoy Bandillo

12.2021

- Published paper in Frontiers of Genetics on genome-wide association study on field pea genetics and phenotyping.
- Performed programming and data analysis for paper.
- doi:10.3389/fgene.2021.707754

Presentations

Applications of High Performance Computing in Precision Agriculture *Fargo, ND*

Stephen Szwiec

04.2024

- Presented a lecture on high performance computing to NDSU precision agriculture students.
- Introduced students to HPC concepts and how these apply to precision agriculture.
- Engaged students in panel discussion on the future of precision agriculture, computational methods, and data science.

Introduction to High Performance Computing *Fargo, ND*

Stephen Szwiec, Sara Tolba

10.2024

- Presented a lecture on high performance computing to NDSU microbiology graduate students.
- Introduced students to HPC concepts, job submission, and parallel programming, and how these apply to life sciences and microbiology.

CCAST Summer 2024 HPC Bootcamp *Fargo, ND*

Nick Dusek, Stephen Szwiec

06.2024

- Developed materials and gave direct support to graduate students in a classroom setting.
- Topics included: HPC basics, job submission, parallel programming, and data analysis.

Python for High Performance Computing *Fargo, ND*

Stephen Szwiec

06.2024

- Diadatic presentation on Python programming for high performance computing for NDSU computer science researchers.
- Developed curriculum and materials for workshop.

Computational Methods for Predicting the Water Permeability of Bio-based Polymer Thermoplastics *Fargo, ND*

Stephen Szwiec, Gerardo Casañola-Martin, Andriy Voronov, Bakhtiyor Rasulev

03.2023

- Poster presentation of new research on computational methods for predicting the water permeability of bio-based polymer thermoplastics presented at the 2023 ND EPSCoR Annual Meeting.

pyQSARplus – A software package for data-driven quantitative structure-activity relationship models

Moorhead, MN

Stephen Szwiec, Bakhtiyor Rasulev

01.2023

- Poster presentation of new QSAR modeling software presented at the 2023 American Chemical Society Red River Valley Section Conference.

Study of Anti-diabetic Properties of Fullerene Derivatives by Application of Molecular Docking and Cheminformatics Methods

Moorhead, MN

Mariam Zamani, Stephen Szwiec, Gerardo Casañola-Martin, Long Nyugen, and Bakhtiyor Rasulev

01.2023

- Poster presentation of new research on possible anti-diabetic nanomedicine presented at the 2023 American Chemical Society Red River Valley Section Conference.

MaterialsBase: A Web-based Tool to Store, Analyze Chemical Data and Design of New Materials

Moorhead, MN

Angel Gallegos, Stephen Szwiec, and Bakhtiyor Rasulev

01.2023

- Poster presentation of new research on a web-based tool for materials design presented at the 2023 American Chemical Society Red River Valley Section Conference.

Predicting Drug-like and Toxicological Properties of Fullerene Derivative Nanostructures by Application of Computational and Machine Learning Approaches

Fargo, ND

Long Nguyen, Stephen Szwiec, Mariam Zamani, Bakhtiyor Rasulev

08.2022

- Poster presentation related to original research of high-throughput docking computational experiment relating fullerene derivatives with diabetes-associated proteins.
- Presented at 2022 NDSU Biomedical REU

Introduction to Data Science and Machine Learning

Fargo, ND

Stephen Szwiec

06.2022

- Three day workshop and didactic presentations on machine learning, applied statistics, and Python programming for NDSU researchers.

Determining Cybersecurity Risk to U.S. Crop Precision Agriculture

Socorro, NM

Stephen Szwiec, Haoying Wang, Jun Zheng

07.2021

- Poster presentation related to data model of cybersecurity exposure and risk to U.S. precision agriculture.
- Presented at REU@NMT CSE 2021.

Projects

CI/CD Framework for High-Performance Computing System

Fargo, ND

North Dakota State University

03.2025 – Present

- Architected reproducible build system using GitHub Actions.
- Researched and developed CI/CD pipelines for improved software deployment and testing.

Non-Fullerene Acceptors for Next-generation Organic Photovoltaics

Fargo, ND

North Dakota State University

10.2024 – Present

- Engineering FAIR-compliant data management platform for collaborative QSPR model development and validation workflows.
- Collecting and curating structural and electronic properties of advanced non-fullerene acceptor molecules.

New Discoveries in the Advanced Interface of Computation, Engineering, and Science (ND-ACES)

Fargo, ND

North Dakota State University

11.2023 – 07.2025

- Provided specialized HPC domain expertise for NSF Award #1946209, supporting computational requirements across multidisciplinary research initiatives.
- Optimized molecular dynamics simulation environments (NAMD, GROMACS, CP2K) for bio-based materials research with architecture-specific performance tuning.

Computational Analysis of Fullerene Derivatives for Organic Photovoltaics
Fargo, ND

North Dakota State University *01.2024 – 10.2024*

- Developed QSPR models integrating chemical descriptors to predict conversion efficiencyof organic photovoltaic devices.
- Performed density functional theory calculations to characterize charge transfer properties of fullerene derivatives.
- Implemented high-throughput computational toxicity screening framework to evaluate biological compatibility of candidate materials.

HPC Infrastructure Modernization Initiative
Fargo, ND

North Dakota State University *05.2023 – 09.2023*

- Orchestrated migration of legacy scientific applications during comprehensive HPC system upgrade cycle.
- Redesigned module environment using Lmod with enhanced logging capabilities and dependency resolution.
- Developed comprehensive technical documentation covering software stack configuration and user-facing interfaces.

Laboratory Knowledge Management System
Fargo, ND

North Dakota State University *07.2022 – 11.2023*

- Established comprehensive digital repository for Computational Polymer Research Group methodologies and procedures.
- Deployed and administered MediaWiki platform with custom extensions for scientific content management and version control.

Parallelized Molecular Docking Framework
Fargo, ND

North Dakota State University *06.2022 – 09.2022*

- Engineered scalable molecular docking pipeline integrating GNU/Parallel with PatchDock and AutoDock Vina for high-throughput screening applications.
- Developed automated post-processing workflow using Perl and shell scripting for analysis of binding site interactions and energetics.

Computational modeling of phase separation in polymers for applications in biofouling release
Fargo, ND

North Dakota State University *01.2022 – 04.2023*

- Developed coarse-grained molecular dynamics models to simulate phase separation dynamics in heterogeneous polymer systems.
- Implemented free energy calculation methods to quantify surface-protein interactions at polymer-water interfaces.
- Integrated simulation results with experimental validation to optimize polymer composition for enhanced biofouling resistance.

High Throughput Genome-wide Association Study of USDA Pea Germplasm
Minot, ND

North Dakota State University *07.2020 – 12.2021*

- Architected scalable bioinformatics pipeline integrating TASSEL5, VCFtools, and R language for GWAS analysis of pea germplasm.
- Deployed OpenStack virtual environment with reproducible configuration management for collaborative genomics research.
- Published findings in peer-reviewed journal, contributing to improved understanding of genetic diversity in pulse crop populations.

Phenotype database audit for pea, chickpea, and lentil experiments
Minot, ND

North Dakota State University *05.2020 – 08.2020*

- Conducted comprehensive audit of two-decade experimental dataset within Agrobase system for pulse crop breeding program.
- Developed MS-SQL analytics scripts incorporating statistical outlier detection and data integrity validation.
- Implemented version-controlled database modification workflow using Trello for task management and Bitbucket for change tracking.

Skills

Programming Languages	Python • C/C++ • Fortran • R • Bash/Shell • Perl • Lua • JavaScript/TypeScript
HPC Software Engineering	MPI • OpenMP • CUDA • Singularity/Apptainer • Lmod • Git • CI/CD
Computational Chemistry	Quantum Chemistry • Molecular Dynamics • Structural Biology • QSPR Modeling

References available upon request.