Dr. Robert J. B. Kalescky

Curriculum Vitae, May 2025

Principal Scientist
Adjunct Professor of Data Science
Southern Methodist University
Dallas, Texas 75205

E-mail: robert@kalescky.org
Phone: (214) 803-1552
GitHub: rkalescky
Publications: ORCiD: 0000-0002-1416-4044
Website: robert.kalescky.org

Research Interests

- Development of scalable machine learning surrogate models for quantum chemical methods
- High-performance implementation of deep learning architectures for analyzing large simulation and experimental datasets
- Data-driven design and screening of functional materials for separations, catalysis, and nano-reactor applications
- Application of graph-based and generative models to accelerate early-stage drug discovery and molecular property prediction
- Optimization of end-to-end computational workflows for materials science and cheminformatics on GPU-accelerated and distributed HPC platforms

Experience

Principal Scientist — May 2024 to May 2025
O'Donnell Data Science and Research Computing Institute
Southern Methodist University, Dallas, Texas

- Directed and developed strategic initiatives and funding opportunities for research computing across disciplines.
- Developed scalable and efficient applications and workflows for chemical simulations and data-intensive machine-learning.

Adjunct Professor of Data Science — May 2020 to Present
Department of Statistics and Data Science
Southern Methodist University, Dallas, Texas

- Designed and taught the Master's of Data Science course HPC and Data Science (DS7347).
- Designed and taught the introduction to data science using Python course (DS1300).
- Taught Master's of Data Science course Quantifying the World (DS7333).

HPC Applications Scientist — May 2015 to May 2024
Office of Information Technology: Research and Data Science Services & Center for Research Computing
Southern Methodist University, Dallas, Texas

- Provided consulting on performance, parallelization, GPU acceleration, and HPC adoption; supported research groups with code migration and optimization across HPC clusters; and mentored faculty and students in computational best practices.
- Instrumental in the procurement, integration, and optimization of ManeFrame II, NVIDIA DGX SuperPOD, and M3 clusters.
- Designed and led HPC and data science courses, workshops, and training sessions for advanced users and researchers.
- SMU President's Award for Innovation (2020) for contributions to computational strategies in COVID-19 campus response.

Postdoctoral Fellow — January 2014 to May 2015
Department of Chemistry Southern Methodist University, Dallas, Texas

- Conducted extensive molecular dynamics simulations and applied the Rigid Residue Scan method to systematically identify key allosteric residues in proteins, enhancing the understanding of intra-protein communication pathways.

Education

Doctor of Philosophy in Chemistry — August 2009 to May 2014
Southern Methodist University, Dallas, Texas
Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes

Master of Science in Chemistry — August 2007 to May 2009
University of Texas at Dallas, Dallas, Texas
Area Per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach

Bachelor of Science in Chemical Engineering, Minors in Mathematics and Chemistry — August 2001 to May 2006
Texas Tech University, Lubbock, Texas
Prairie Grass Ethanol Production Pilot Plant Facility and Optimization

Core Competencies and Technical Expertise

Machine Learning	Scientific machine learning with PyTorch, TensorFlow, PyTorch Geometric (PyG), GPyTorch, and scikit-learn; model development on large datasets
Data Science Tools	Jupyter, RStudio, scikit-learn, RAPIDS
High-Performance Computing	Parallel and distributed algorithms, application scaling and optimization, GPU acceleration
Programming Languages	Python, C, C++, Fortran, Rust, Julia, Objective-C, R
Scientific Development	Performance tuning, code migration, HPC adoption, and best-practices development
Parallelism	MPI, OpenMP, CUDA, OpenCL, Pthreads, (Open|NV)SHMEM, KOKKOS, RAJA, OCCA, NCCL
Containerization	Docker, Singularity, Apptainer, Enroot
Documentation	LaTeX, BibTeX, reStructuredText, Sphinx, Markdown, MediaWiki, HTML
IDEs and Portals	Jupyter, RStudio, Open OnDemand HPC Portal
Source Control	Git, Mercurial, Subversion
Collaboration	Project management, interdisciplinary research consulting, team mentoring
Application Areas	Quantum chemistry, molecular dynamics, materials science, drug discovery, and machine learning
Libraries	Armadillo, Eigen, PyTorch, PyTorch Geometric (PyG), GPyTorch, HPC SDK
Molecular Modeling	Gaussian, CFOUR, Q-Chem, GAMESS, PySCF, DFTB+, Molpro, NWChem, DIRAC, ORCA, GPAW, Columbus, ABINIT
Molecular Dynamics	CHARMM, NAMD, LAMMPS, Amber, MPDyn, GROMACS, OpenMM
Calculation Types	Optimized geometries, transition states, reaction paths, potential energy surfaces, spectroscopic data, binding free energies
Visualization	VMD, Chimera, Avogadro, IQmol, POV-Ray
Scripting	Bash, CSH, AWK, Perl, sed, Tcl
Administration	UNIX system administration on Linux (Red Hat/Debian), macOS, FreeBSD, and Solaris

Publications

(19) Green, K.; Casler, C.; Deumens, E.; Jezghani, A.; Kalescky, R.; Kelley, K.; Michael, S.; Hanna, E.; MacLachlan, G.; Stanzione, D.; Coulter, E. *Energy Efficiency in Research Data Centers*; tech. rep., Whitepaper on energy efficiency challenges and solutions for research data centers.; Coalition for Academic Scientific Computation (CASC), 2024.

(18) Delgado, A. A. A.; Humason, A.; Kalescky, R.; Freindorf, M.; Kraka, E. Exceptionally Long Covalent CC Bonds—A Local Vibrational Mode Study. *Molecules* **2021**, *26*, DOI: 10.3390/molecules26040950.

(17) Kalescky, R.; Zhou, H.; Liu, J.; Tao, P. Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery. *PLoS Comput Biol* **2016**, *12*, 1–21.

(16) Neeman, H.; Bergstrom, A.; Brunson, D.; Ganote, C.; Gray, Z.; Guilfoos, B.; Kalescky, R.; Lemley, E.; Moore, B. G.; Ramadugu, S. K.; Romanella, A.; Rush, J.; Sherman, A. H.; Stengel, B.; Voss, D. In *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*, ACM: Miami, USA, 2016, 57:1–57:8.

(15) Setiawan, D.; Kalescky, R.; Kraka, E.; Cremer, D. Direct Measure of Metal–Ligand Bonding Replacing the Tolman Electronic Parameter. *Inorganic Chemistry* **2016**, *55*, 2332–2344.

(14) Kalescky, R.; Liu, J.; Tao, P. Identifying Key Residues for Protein Allostery through Rigid Residue Scan. *The Journal of Physical Chemistry A* **2015**, *119*, 1689–1700.

(13) Kalescky, R.; Kraka, E.; Cremer, D. Accurate determination of the binding energy of the formic acid dimer: The importance of geometry relaxation. *The Journal of Chemical Physics* **2014**, *140*, DOI: http://dx.doi.org/10.1063/1.4866696.

(12) Kalescky, R.; Kraka, E.; Cremer, D. Are carbon—halogen double and triple bonds possible? *International Journal of Quantum Chemistry* **2014**, *114*, 1060–1072.

(11) Kalescky, R.; Kraka, E.; Cremer, D. Description of Aromaticity with the Help of Vibrational Spectroscopy: Anthracene and Phenanthrene. *The Journal of Physical Chemistry A* **2014**, *118*, 223–237.

(10) Kalescky, R.; Kraka, E.; Cremer, D. New Approach to Tolman's Electronic Parameter Based on Local Vibrational Modes. *Inorganic Chemistry* **2014**, *53*, 478–495.

(9) Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Quantitative Assessment of the Multiplicity of Carbon–Halogen Bonds: Carbenium and Halonium Ions with F, Cl, Br, and I. *The Journal of Physical Chemistry A* **2014**, *118*, 1948–1963.

(8) Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Vibrational Properties of the Isotopomers of the Water Dimer Derived from Experiment and Computations. *Australian Journal of Chemistry* **2014**, *67*, 426–434.

(7) Kalescky, R.; Kraka, E.; Cremer, D. Local vibrational modes of the formic acid dimer – the strength of the double hydrogen bond. *Molecular Physics* **2013**, *111*, 1497–1510.

(6) Kalescky, R.; Kraka, E.; Cremer, D. Identification of the Strongest Bonds in Chemistry. *The Journal of Physical Chemistry A* **2013**, *117*, 8981–8995.

(5) Zou, W.; Kalescky, R.; Kraka, E.; Cremer, D. Relating normal vibrational modes to local vibrational modes: benzene and naphthalene. *Journal of Molecular Modeling* **2013**, *19*, 2865–2877.

(4) Kalescky, R.; Zou, W.; Kraka, E.; Cremer, D. Local vibrational modes of the water dimer – Comparison of theory and experiment. *Chemical Physics Letters* **2012**, *554*, 243 –247.

(3) Zou, W.; Kalescky, R.; Kraka, E.; Cremer, D. Relating normal vibrational modes to local vibrational modes with the help of an adiabatic connection scheme. *The Journal of Chemical Physics* **2012**, *137*, DOI: http://dx.doi.org/10.1063/1.4747339.

(2) Udayana Ranatunga, R. J. K.; Kalescky, R. J. B.; Chiu, C.-c.; Nielsen, S. O. Molecular Dynamics Simulations of Surfactant Functionalized Nanoparticles in the Vicinity of an Oil/Water Interface. *The Journal of Physical Chemistry C* **2010**, *114*, 12151–12157.

(1) Kalescky, R. J. B.; Shinoda, W.; Moore, P. B.; Nielsen, S. O. Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach. *Langmuir* **2009**, *25*, 1352–1359.

Conference Presentations

(15) Introduction to Data Resources, Presentation, Think-Play-Hack — World Views, 2019.

(14) Evaluation of DFT Dispersion Corrections on Hydrogen Isotopologue Separation in Metal-Organic Frameworks, Presentation, Austin Symposium of Molecular Structure and Dynamics, 2018.

(13) Hydrogen Isotopologue Separation in CPO-27-X, Poster, Austin Symposium of Molecular Structure and Dynamics, 2018.

(12) Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes, Presentation, Southern Methodist University, Department of Chemistry, 2014.

(11) Using Rigid Body Molecular Dynamics to Explore Key Residues of Protein Allostery, Presentation, Southwest Regional Meeting of the American Chemical Society, 2014.

(10) What are the Strongest Bonds in Chemistry, Poster, Austin Symposium of Molecular Structure and Dynamics, 2014.

(9) A Force Field for the Study of Small Molecule Absorption and Diffusion By Metal-Organic Frameworks in Fully Flexible Simulations, Presentation, Southern Methodist University, Department of Chemistry, 2013.

(8) Description of the Strength of Carbon-Halogen and Carbon-Chalcogen Bonds Utilizing Local Vibrational Modes, Presentation, Chirality, 2012.

(7) Exotic Carbon-Halogen Bonds Described By Local Vibrational Modes, Poster, Austin Symposium of Molecular Structure and Dynamics, 2012.

(6) Description of the Strength of Carbon-Halogen and Carbon-Chalcogen Bonds Utilizing Local Vibrational Modes, Presentation, Southern Methodist University, Department of Chemistry, 2011.

(5) Carbon Nanotubes: Structure, Properties, and Controlled Synthesis, Presentation, Southern Methodist University, Department of Chemistry, 2010.

(4) Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach, Presentation, University of Texas at Dallas, Department of Chemistry, 2009.

(3) Area per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach, Poster, Chem-Bio Symposium, 2008.

(2) Correlating Surfactant Hydrophilic-Lipophilic Balance and Nanoparticle Radii via Coarse-Grained Molecular Dynamics Simulations, Presentation, Dallas/Fort Worth Local American Chemical Society Meeting, 2008.

(1) Correlating Surfactant Hydrophilic-Lipophilic Balance and Nanoparticle Radii via Coarse-Grained Molecular Dynamics Simulations, Presentation, American Chemical Society, 2008.

Conferences and Workshops Attended

(28) Coalition for Academic Scientific Computation Meeting, Arlington, Virginia, U.S. 2023.

(27) SMU CAPE Project Management Certificate Program, Dallas, Texas, U.S. 2023.

(26) Super Computing 2023, Denver, Colorado, U.S. 2023.

(25) Coalition for Academic Scientific Computation Meeting, Alexandria, Virginia, U.S. 2022.

(24) NVIDIA GPU Technology Conference, Virtual Conference, 2022.

(23) Super Computing 2022, Dallas, Texas, U.S. 2022.

(22) Super Computing 2021, Virtual Conference, 2021.

(21) Super Computing 2020, Virtual Conference, 2020.

(20) Coalition for Academic Scientific Computation Meeting, Alexandria, Virginia, U.S. 2019.

(19) Super Computing 2019, Denver, Colorado, U.S. 2019.

(18) Think-Play-Hack — World Views, Taos, New Mexico, U.S. 2019.

(17) Austin Symposium of Molecular Structure and Dynamics, Dallas, Texas, U.S. 2018.

(16) Super Computing 2018, Dallas, Texas, U.S. 2018.

(15) Super Computing 2017, Denver, Colorado, U.S. 2017.

(14) Advanced Cyber Infrastructure – Research and Educatation Facilitators, University of Oklahoma, Norman, Oklahoma, U.S. 2016.

(13) International Conference on Computational Science (ICCS), University of California at San Diego and San Diego Supercomputer Center (SDSC), San Diego, California, U.S. 2016.

(12) S2SI High-Energy Physics and Computer Science, University of Illinois at Urbana–Champaign, Urbana and Champaign, Illinois, U.S. 2016.

(11) Super Computing 2016, Salt Lake City, Utah, U.S. 2016.

(10) Advanced Cyber Infrastructure – Research and Educatation Facilitators, University of Oklahoma, Norman, Oklahoma, U.S. 2015.

(9) Super Computing 2015, Austin, Texas, U.S. 2015.

(8) Austin Symposium of Molecular Structure and Dynamics, Dallas, Texas, U.S. 2014.

(7) Southwest Regional Meeting of the American Chemical Society, Fort Worth, Texas, U.S. 2014.

(6) Austin Symposium of Molecular Structure and Dynamics, Dallas, Texas, U.S. 2012.

(5) Chirality 2012, Fort Worth, Texas, U.S. 2012.

(4) 242nd American Chemical Society National Meeting, Denver, Colorado, U.S. 2011.

(3) 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S. 2008.

(2) Chem-Bio Symposium, University of Texas at Dallas, Dallas, Texas, U.S. 2008.

(1) Dallas/Fort Worth Local American Chemical Society Meeting, Southern Methodist University, Dallas, Texas, U.S. 2008.

Invited Seminar Presentations

(7) Introduction to High Performance Computing, ManeFrame, and Applications, Presentation, Southern Methodist University, Department of Computer Science and Engineering, Graduate Seminar, 2019.

(6) Using Jupyter Lab on M2, Presentation, Southern Methodist University, Department of Computer Science and Engineering, 2018.

(5) Accelerated Computations on ManeFrame II, Presentation, Southern Methodist University, Department of Computer Science and Engineering, Graduate Seminar, 2017.

(4) Supercomputing at SMU: An Introduction to ManeFrame, Presentation, Southern Methodist University, Department of Statistical Science, Graduate Seminar, 2017.

(3) Introduction to High Performance Computing, ManeFrame, and Applications, Presentation, Southern Methodist University, Department of Computer Science and Engineering, Graduate Seminar, 2016.

(2) ManeFrame Introduction, Presentation, Southern Methodist University, Department of Physics, Graduate Seminar, 2016.

(1) ManeFrame Introduction for Economics, Presentation, Southern Methodist University, Department of Economics, Graduate Seminar, 2016.

Teaching

2024

- DS 7333: Quantifying the World

2023

- DS 1300: A Practical Introduction to Data Science
- DS 7347: Data Science and High-Performance Computing

2022

- DS 1300: A Practical Introduction to Data Science
- DS 7347: Data Science and High-Performance Computing

2021

- DS 1300: A Practical Introduction to Data Science

Technical Workshops

2025

- O'Donnell Data Science and Research Computing Institute — 2 2-hour workshops
  1. Distributed Python 2. Graph Machine Learning Fundamentals

2024

- O'Donnell Data Science and Research Computing Institute — 2 2-hour workshops
  1. Introduction to HPC 2. Parallel Programming in C++

2023

- Research and Data Science Services Workshop Series — 3 2-hour workshops
  1. Introduction to HPC 2. Scaling HPC Workflows 3. Kubernetes for Beginners

2022

- Research and Data Science Services Workshop Series — 5 2-hour workshops
  1. C++ Parallel STL 2. KOKKOS & RAJA 3. MPL (Modern C++ MPI) 4. R libraries from C++ 5. Python modules from C++
- Speed Data-ing

2021

- Center for Research Computing Spring Workshop Series — 9 2-hour workshops
  1. ManeFrame II (M2) Introduction 2. Intel oneAPI HPC Toolkit Overview 3. Python Workflows on ManeFrame II (M2) 4. NVIDIA HPC SDK Overview 5. ManeFrame II (M2) Introduction 6. R Workflows on ManeFrame II (M2) 7. Introduction to OpenMP and OpenACC 8. Introduction to MPI 9. Introduction to Standard C++ Parallel Algorithms

2020

- Center for Research Computing Fall Workshop Series — 11 2-hour workshops
  1. M2 Introduction & New Storage Workflow 2. Python Workflows on M2 3. R Workflows on M2 4. Julia Workflows on M2 5. Docker & Singularity on M2 6. M2 Introduction & New Storage Workflows 7. Introduction to MPI 8. Introduction to OpenMP 9. Introduction to OpenACC 10. M2 Introduction & New Storage Workflows 11. Introduction to Standard C++ Parallel Algorithms
- Center for Research Computing Summer Workshop Series — Five full-day workshops
- Center for Research Computing Spring Workshop Series — 14 2-hour workshops
  1. M2 Introduction 2. Introduction to LAPACK and BLAS 3. Text Mining with Python on M2 4. Using the New HPC Portal 5. Using GitHub 6. Writing Portable Accelerator Code with KOKKOS, RAJA, and OCCA 7. M2 Introduction 8. Introduction to Parallelization Using MPI 9. Writing High Performance Python Code 10. Creating Portable Environments with Singularity and Docker 11. M2 Introduction 12. Introduction to Parallelization Using OpenMP and OpenACC 13. Profiling Applications on M2 14. Improving Code Vectorization

2019

- Center for Research Computing Fall Workshop Series — 12 2-hour workshops
  1. Introduction to Using M2 2. Vectorization Using OpenMP 3. R Workflows on M2 4. Using Git and GitHub 5. Introduction to Using M2 6. Python Workflows on M2 7. Hybrid MPI with OpenMP and OpenACC 8. Using Machine Learning Toolkits on M2 9. Parallel Architecture Abstraction Via OCCA and RAJA 10. Introduction to Using M2 11. Using Docker and Singularity on M2 12. Introduction to Using M2
- Center for Research Computing Summer Workshop Series — Week-long, full-day workshop
- Center for Research Computing Spring Workshop Series — 12 2-hour workshops
  1. ManeFrame II (M2) Introduction 2. Open Help Session 3. ManeFrame II (M2) Introduction 4. Using Version Control 5. Using Spack for Development 6. ManeFrame II (M2) Introduction 7. Using Accelerated Libraries 8. ManeFrame II (M2) Introduction 9. Improving Vectorization 10. Using MPI + OpenMP/OpenACC 11. Open Help Session 12. ManeFrame II (M2) Introduction

2018

- Center for Scientific Computation Fall Workshop Series — 14 2-hour workshops
  1. ManeFrame II (M2) Introduction 2. Open Help Session 3. ManeFrame II (M2) Introduction 4. Parallel R on M2 5. Using Spack for Development 6. Open Help Session 7. ManeFrame II (M2) Introduction 8. OpenMP Introduction 9. OpenACC Introduction 10. MPI Introduction 11. Open Help Session 12. ManeFrame II (M2) Introduction 13. Parallel Python on M2 14. Open Help Session
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop
- Center for Scientific Computation Spring Workshop Series — 14 2-hour workshops
  1. Introduction to ManeFrame II (M2) 2. Using R on ManeFrame II (M2) 3. Introduction to ManeFrame II (M2) 4. Using SAS on ManeFrame II (M2) 5. Introduction to Jupyter Notebooks 6. Accessing Graphical Applications on ManeFrame II (M2) 7. Introduction to ManeFrame II (M2) 8. Using the NVIDIA P100 Nodes 9. Advanced Slurm Features 10. Introduction to ManeFrame II (M2) 11. Using the Intel Xeon Phi Nodes 12. Parallel Python on ManeFrame II (M2) 13. Tips for Automating Computational Workflows
- Mathworks MATLAB Workshop — 3-hour workshop

2017

- Center for Scientific Computation Fall Workshop Series — 10 2-hour workshops
  1. Migrating to ManeFrame II 2. Introduction to ManeFrame II 3. Debugging Python 4. Parallel Python 5. Introduction to Jupyter Notebooks 6. Porting Applications to MICs and GPUs 7. Introduction to ManeFrame II 8. Debugging Parallel Applications with Allinea DDT 9. Profiling Parallel Applications with Allinea MAP 10. Introduction to ManeFrame II
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop
- Center for Scientific Computation Spring Workshop Series — 13 3-hour workshops
  1. Introduction to Parallel Computing 2. Introduction to Research Programming 3. Introduction to Parallel Programming 4. Introduction to Research Computing 5. Introduction to Vectorization 6. Introduction to Shared-Memory Parallel Programming 7. Introduction to Distributed-Memory Parallel Programming 8. Introduction to Research Computing 9. Introduction to Accelerator Programming 10. OpenMP Deep Dive 11. MPI Deep Dive 12. Introduction to Research Computing 13. CUDA and OpenCL Deep Dive

2016

- Center for Scientific Computation Fall Workshop Series — 9 3-hour workshops
  1. Open Help Session 2. ManeFrame Introduction 3. GPGPU Development on ManeFrame 4. Introduction to Jupyter 5. Open Help Session 6. ManeFrame Introduction 7. Debugging and Profiling Parallel Applications on ManeFrame 8. ManeFrame Introduction 9. Introduction to Build Automation Development Tools
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop
- Center for Scientific Computation Spring Workshop Series — 7 3-hour workshops
  1. Introduction to Using ManeFrame 2. Introduction to Julia 3. Python in HPC Environment 4. Parallel Programming on ManeFrame 5. GPGPU Programming Overview 6. OpenCL for HPC 7. Using R on ManeFrame

2015

- Center for Scientific Computation Fall Workshop Series — 6 3-hour workshops
  1. Introduction to Using ManeFrame 2. Introduction to Parallel Programming 3. Post-processing Data Using Python 4. Bash Shell Scripting 5. Introduction to C++ MPI Programming 6. Introduction to GPGPU Programming
- Center for Scientific Computation Summer Workshop — Week-long, full-day workshop

2014

- Advanced Python Programming Workshop — Fall 2014
- Advanced CHARMM Workshop — Spring 2014
- CATCO URVA Workshop

2013

- Graduate/Undergraduate Computational Chemistry Laboratory
- LaTeX Workshop — Spring 2013

2012

- Graduate/Undergraduate Computer Aided Drug Design Laboratory
- CATCO Methods Workshop

- CATCO URVA Workshop

2011

- Graduate/Undergraduate Computational Chemistry Laboratory

2010

- Graduate/Undergraduate Computer Aided Drug Design Laboratory
- Undergraduate General Chemistry Laboratory

2009

- Graduate/Undergraduate Computational Chemistry Laboratory

Student Advisement

Graduate

- Robert Ortega, Southern Methodist University
  - Performance tuning of parallel free energy sampling methods — September 2020 to May 2021

Undergraduate

- Gabriel Mongaras, Southern Methodist University
  - Describing electron density through machine learning models — August 2022 to December 2023
- Carter Koehler, Southern Methodist University
  - Describing electron density through machine learning models — August 2018 to December 2018
  - Super Computing 2018 Student Cluster Competition — January 2018 to May 2018
- Ethan Britt, University of Texas at Dallas — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Mauhib Iqbal, University of Texas at Dallas — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Boce Lin, Southern Methodist University — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Rick Simon, Southern Methodist University — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Vyas Nellutla, University of Texas at Dallas — January 2018 to May 2018
  - Super Computing 2018 Student Cluster Competition
- Moez Janmohammad, Southern Methodist University — January 2016 to May 2016
  - Engaged Learning Big iDeas Project
  - ARM Beowulf cluster prototype

University Activities and Committees

- Southern Methodist University Enterprise Architecture Board (EAB) Chair-Elect — August 2023 to May 2024
- Southern Methodist University Enterprise Architecture Board (EAB) — June 2021 to May 2024
- COVID-19 Spring 2021 academic facilities allocation taskforce (*Data Ninjas* for Operations "Room of Requirement" and "Sorting Hat") for the Southern Methodist University Office of Information Technology and Administration — September 2020 to Present
- COVID-19 Fall 2020 academic facilities allocation taskforce (*Data Ninjas* for Operations "Room of Requirement" and "Sorting Hat") for the Southern Methodist University Office of Information Technology and Administration — May 2020 to August 2020
- Member of campus-wide Clowder implementation group — February 2020 to Present
- Member of Open On-Demand HPC Portal implementation group — April 2019 to December 2019
- Search committee member for the Southern Methodist University Office of Information Technology Data Science Consultant hire — 2018
- Search committee member for the Southern Methodist University Office of Information Technology HPC Consultant hire — 2018
- Search committee member for the Southern Methodist University Office of Information Technology Senior HPC Systems Administrator hire — 2017
- Member of core group tasked with the planning, design, acquisition, and implementation of Southern Methodist University's ManeFrame II (M2) cluster — 2016 to 2017

Service and Outreach

- SMU Reads Facilitator, *Lab Girl* by Hope Jahren — Fall 2018
- Led Southern Methodist University and University of Texas at Dallas joint team application to the Super Computing 2018 Student Cluster Competition — Spring 2018
- Designed book cover image for *Fundamentals of Controlled/Living Radical Polymerization*; Tsarevsky, N. V.; Sumerlin, B. S., Eds.; The Royal Society of Chemistry, 2013; pp. P001–P364.
- Graduate Student Assembly Representative (Southern Methodist University, Department of Chemistry) — August 2011 to August 2013
- Introduction to Computational Chemistry for High School Instructors — 2011
- Graduate Student Symposium Planning Committee Member (American Chemical Society) — Fall 2011
- Chemistry Graduate Council Treasurer (Southern Methodist University) — 2011
- American Chemical Society Graduate Student Symposium Planning Committee — Spring 2011
- Chemistry Graduate Council Secretary (Southern Methodist University) — 2010

Merits

Certificates

- Project Management Certificate, Southern Methodist University — December 2023

Awards and Honors

- President's Award for Innovation, Southern Methodist University — October 20, 2020
- 1st Place Poster Competition for Chemistry, Research Day, Southern Methodist University — February 10, 2012
- 2nd Place Poster Competition, Chem-Bio Symposium, University of Texas at Dallas — March 26, 2008
- Four-year varsity letterman; co-captain of the Texas Tech cross country and track teams — August 2001 to May 2005
- Recognized by Texas Tech University and the Big 12 Conference for excellence as a student athlete