Christopher A. Myers, PhD

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Computational Scientist Overview

- parameterized models with chemistry-based datasets for scientific research.
- Highly skilled in scientific software development for high-performance computing environments.
- Proven leader in mentoring junior and senior scientists in developing computational solutions to a wide array of scientific problems, including collaborations with experimental laboratories.

Education

PhD, Physics, 2022
Master of Science, Physics, 2017
University at Albany (SUNY), Albany, NY

- PhD Dissertation: "Turning density functional theory calculations into molecular mechanics simulations: Establishing the fluctuating density model for RNA nucleobases".

Bachelor of Science, Physics, 2014
University at Albany (SUNY), Albany, NY

Project Management

Program Manager | U.S. Department of Energy

January 12, 2025 – February 13 2025 | Office of Science | Advanced Scientific Computing Research (ASCR)
19901 Germantown Rd, Germantown, MD 20874

- Managed HPC resource allocations for national laboratory, industrial, and academic research projects for the ASCR Leadership Computing Challenge (ALCC).
- Oversaw proposal evaluations and stakeholder engagement to advance DOE's scientific computing initiatives.
- Strategized future allocation projects, including Integrated Research Infrastructure (IRI), and scientific communications to enhance program outreach and research impact.

Research and Model Development Experience

Postdoctoral Researcher | University of California, Merced | Full Time

November 1**,** 2022 - January 10, 2025 | Department of Chemistry & Biochemistry
5200 Lake Rd, Merced, CA 95343

Data Science and Model Parameterization

- Spearheaded our group's efforts to improve the performance of molecular dynamics simulations with neural networks, nonlinear regression, and clustering algorithms.
  - PyTorch, Scikit-learn, SciPy, and Pandas libraries, and implemented various molecular descriptors.
- Improved the accuracy of mixed QM/MM chromophore-solvent force fields, resulting in the reproduction of UV-Vis, Raman, and nonlinear optical spectra from experiments.
- Parameterized force fields from electronic structure data sets to study Förster resonance energy transfer (FRET) and optical cavity polariton experiments.

Scientific Programming

- Developed production-grade Python software that links novel nonadiabatic dynamics simulation algorithms with a commercial GPU quantum chemistry program through a server-client model.
- Accelerated in-house UV-Vis spectroscopy software for high-performance computing environments by parallelizing simulation workloads: achieved over a tenfold speedup.
- Trained colleagues through oral presentations and tutorials in strategies for improving Python efficiency and documenting code development with Git and GitHub.

Project Organization and Collaboration

- Held a leading role on multiple concurrent research projects and partnered with both experimental & computational labs outside the university to corroborate measurements with predicted outcomes.
- Mentored a diverse group of student researchers on machine learning and optimization fundamentals, and aligned project directions with their expertise, interests, and graduation goals.
- Presented project results at conferences and monthly meetings with collaborators across the country.

Graduate Research Assistant | University at Albany (SUNY) | Full Time

June 1, 2017-October 30, 2022 **|** Chemistry Department and The RNA Institute
1400 Washington Avenue Albany, NY 12222

Biochemistry and Materials Chemistry Collaborations

- Developed multi-threaded C++ code to simulate ion mobility mass spectrometry experiments studying the structure of nucleic acids and proteins.
  - Resulted in a peer-reviewed publication and outperformed multiple competing software.
- Published a review article on the challenges of simulating modified RNA nucleotides from both a computational and experimental perspective.
- Developed force fields to simulate nucleic acids interacting with graphene biosensing devices.
- Corroborated experimental outcomes with DFT computations to deduce chemical degradation mechanisms of 2D materials and coordination of ligand protectants.

RNA Molecular Dynamics

- Constructed a novel polarizable molecular mechanics model for RNA nucleobases, deployed as a combined C++/Python add-on for the OpenMM simulation library.
- Implemented a protocol for scheduling replica exchange MD simulations of tRNA folding pathways.
- Parameterized force fields for RNA, small molecules, and newly synthesized organic molecules from *ab initio* DFT computations.
- Experience with free energy calculations using umbrella sampling/integration and free energy perturbation methods.

Graduate Research Assistant | University at Albany (SUNY)

June 1, 2014-May 31, 2017 **|** Physics Department
1400 Washington Avenue Albany, NY 12222

Electron Spin Resonance Spectroscopy

- Constructed a Brownian motion-based model to replicate ESR spectra from classical molecular dynamics simulations.
- Developed Java code with a graphical user interface to calculate and compare experimental and computational ESR data

Skills and Technical Abilities

Algorithms and Data Analysis: Numerical optimization, model parameterization, numerical integration, linear algebra, statistical analysis and data visualization. Experience with neural networks, linear and nonlinear regression, data curation procedures, and general machine learning fundamentals.

Programing Languages: Advanced fluency in Python and C++. Experience with C, C#, Java, Matlab, Bash (Linux), Mathematica, LaTeX, OpenMP and multiprocessing techniques.

Molecular Dynamics: free-energy perturbation, umbrella sampling and integration, replica exchange simulations, fixed-charge and polarizable force field development (AMBER, CHARMM, OPLS), nucleic acid and protein simulations, mixed QM/MM simulations. AMBER, OpenMM, and GROMACS software.

Quantum Chemistry: Density Functional Theory (DFT), Time Dependent DFT, Plane Wave DFT, UV-Vis absorption spectroscopy, FRET, nonadiabatic simulations, optical cavity spectroscopy. TeraChem, Q-Chem, Quantum Espresso, Gaussian, DFTB+, Psi4 and CP2K Software.

Teaching Experience

Graduate Teaching Assistant, 2014-2017
University at Albany (SUNY), Physics Department

- Prepared lecture material for Physics I and II supplemental discussion classes for 30-60 students/semester.
- Created practice exam problems and instructed review sessions for 100+ student audiences.
- Instructed weekly laboratory classes and graded lab reports, exams, and quizzes.

Awards and Acknowledgments

Excellence in Research
- Awarded by University at Albany Physics Department, Spring 2016 on the merits of exceptional research abilities.

Best Presentation at the PASCAL conference, Albany NY,
- Awarded by University at Albany Physics Department, Spring 2016.

Publications

1) **Christopher A. Myers**, Ken Miyazaki, Thomas Trepl, Christine M. Isborn, and Nandini Ananth. "GPU-Accelerated On-the-fly Nonadiabatic Semiclassical Dynamics". *J. Chem. Phys. 161, 084114 (2024).*

2) **Christopher A. Myers**, Shao-Yu Lu, Sapana Shedge, Arthur Pyuskulyan, Katherine Donahoe, Liang Shi, Christine M. Isborn. "Axial H-bonding Solvent Controls Inhomogeneous Spectral Broadening, Peripheral H-bonding Solvent Controls Vibronic Broadening: Cresyl Violet in Methanol." *J. Phys. Chem. B* 2024, 128, 23, 5685–5699.

3) **Christopher A. Myers**, Alan A. Chen. "A Fluctuating Density Energy Model for RNA Nucleobase Interactions." *ChemRxiv* 10.26434/chemrxiv-2023-1rvh3, 2023.

4) Biswas, Samadrita; Kaur, Simi; **Myers, Christopher**; Chen, Alan; Welch, John. "Aggregation in aqueous solutions of 2-(tetrafluoro(trifluoromethyl)-λ6-sulfanyl-ethan-1-ol (CF3SF4-ethanol): A comparison with aqueous trifluoroethanol and hexafluoroisopropanol using molecular dynamics simulations and dynamic light scattering experiments." *ACS Omega*, 2023, 8, 33, 30037.

5) Mengwen Yan, **Christopher A. Myers**, Gregory M. John, Vincent E. Meyers, Alan A. Chen, Jeremy I. Feldblyum. "Probing the Edges between Stability and Degradation of a Series of ZnSe-Based Layered Hybrid Semiconductors." *Adv. Mater. Interfaces* 2022, 9, 2200347.

6) Rebecca J. D'Esposito, **Christopher A. Myers**, Alan A. Chen, and Sweta Vangaveti. "Challenges with simulating modified RNA: Insights into role and reciprocity of experimental and computational approaches." *Genes* 2022*,* 13, 540.

7) **Christopher A. Myers**, Rebecca J. D'Esposito, Daniele Fabris, Srivathsan V. Ranganathan, Alan A. Chen. "CoSIMS: A Collision Simulator for Ion Mobility Spectrometry." *J. Phys. Chem. B* 2019, 123, 20, 4347–4357.

8) Srivathsan V. Ranganathan, Ken Halvorsen, **Christopher A. Myers**, Neil M. Robertson, Mehmet V. Yigit, Alan A. Chen. "Complex Thermodynamic Behavior of Single-Stranded Nucleic Acid Adsorption to Graphene Surfaces." *Langmuir* 2016, 32, 24, 6028–6034.

Conference Presentations

1) Christopher A. Myers, Ken Miyazaki, Thomas Trepl, Nandini Ananth, and Christine M. Isborn, "On-the-fly Semiclassics for Large Systems: Implementation of LSC-IVR with TeraChem". Poster presented at 2024 West Coast Theoretical Chemistry Meeting, Merced, CA.

2) Christopher A. Myers, Shao-Yu Lu, Sapana Shedge, Arthur Pyuskulyan, Katherine Donahoe, Liang Shi, and Christine M. Isborn. "Constructing a Solute-Solvent Force Field from ab initio Calculations for Spectral Lineshape Prediction: A Cresyl Violet Story." 2024. Oral presentation at American Chemical Society, Spring 2024.

3) Christopher A. Myers, Shao-Yu Lu, Sapana Shedge, Arthur Pyuskulyan, Katherine Donahoe, Liang Shi, and Christine M. Isborn. The Interplay Between Solute-Solvent Interactions for Spectral Lineshapes of the Cresyl Violet Chromophore. 35th Workshop on Recent Developments in Electronic Structure Methods, UC Merced, 2023.

4) Christopher A. Myers, Aleksey A. Kocherzhenko, Sapana V. Shedge, and Christine M. Isborn. Modeling the Effects of Disorder of Opical Cavity Ensembles. Poster presented at Strong Coupling of Organic Molecules 2023 (SCOM23) international conference, La Jolla, CA.

5) Christopher A. Myers, Shao-Yu Lu, Sapana Shedge, Arthur Pyuskulyan, Liang Shi, and Christine M. Isborn. The Interplay Between Solute-Solvent Interactions for Spectral Lineshapes of the Cresyl Violet Chromophore. Poster presented at 2023 West Coast Theoretical Chemistry Meeting, Davis, CA.

6) Christopher A. Myers, Alan A. Chen. Simulations in charge of their own electrostatics: Augmenting a nucleic acid force field with fluctuating charge densities. Oral presentation at American Chemical Society, Spring 2022 and poster presentation American Physical Society March Meeting, 2022.

7) Christopher A. Myers, Alan A. Chen. A Potential Improvement for Electrostatic Interactions: Constructing A Fluctuating Charge Model for Nucleic Acids. Oral presentation at American Physical Society, March Meeting 2021.

8) Christopher A. Myers, Rebecca D'Esposito, Alan A. Chen. A Fluctuating Charge Model for Gas Phase Nucleic Acid Simulations. Virtual poster presented at American Chemical Society, Fall 2020.

9) Christopher A. Myers, Rebecca D'Esposito, Alan A. Chen. From Density Functional Theory to Molecular Mechanics: A Fluctuating Charge model for DNA and RNA. Oral presentation to the Physics Department, University at Albany, NY, 2020.

10) Christopher A. Myers, Rebecca J. D'Esposito, Alan A. Chen, Accounting for Electrostatic Polarization in Gas-Phase Simulations of Ion Mobility Spectrometry. Oral presentation at Molecular Biophysics in the Northeast 2019, Boston, Massachusetts.

11) Christopher A. Myers, Alan A. Chen. Construction of a Dynamic-Charge Model for Gas Phase Simulations of Ion Mobility Spectrometry. Poster presented at Albany 2019: The 20th Conversation, Albany New York, 2019.

12) Christopher A. Myers, Alan A. Chen. Where do Charges Come From? A Deconstruction of MD Force Field Electrostatics. Oral presentation at the PASCAL, Albany New York, 2018.

13) Christopher A. Myers, Alan A. Chen, Keith A. Earle. Simulating Electron Spin Resonance Experiments with Brownian Dynamics. Poster presented at the Telluride School on Time-Dependent Density Functional Theory, 2017.

14) Christopher A. Myers, Keith Earle, Alan A. Chen. Simulating and Interpreting Electron Spin Resonance and Ion Mobility Experiments. Oral presentation to the Physics Department, University at Albany, NY, 2017.

15) Christopher A. Myers, Keith A. Earle. Parameter Inference from Molecular Dynamics Informed Lineshape Calculations. Poster presented at the 36th Annual International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering, Ghent, Belgium, 2016.

16) Christopher A. Myers, Keith A. Earle, Srivathsan V. Ranganathan, Sweta Vangaveti, Alan A. Chen. A New Trajectory Method for Calculating Collision Cross-Sections of Nucleic Acids. Oral and poster presentation presented at the PASCAL, Albany, New York, 2016.

17) Srivathsan V. Ranganathan, Christopher A. Myers, Ken Halvorsen, Neil M. Robertson, Mehmet V. Yigit, and Alan A. Chen. Modeling Nucleic Acid Behavior at Graphene-Water Interfaces for Applications in Bio-sensing & Drug Delivery. Poster presented at the 59th Annual Meeting of the Biophysical Society, Baltimore, Maryland, 2015.