

Michele Myong, PhD

Dallas-Fort Worth Metropolitan Area | michele.myong@gmail.com | [Website](#) | [LinkedIn](#) | [Github](#)

SUMMARY

I am a Physical Chemist and Scientific Programmer with 9 years of experience in laser science, optical materials, and renewable energy research, using complex analysis and modeling to measure novel materials for clean energy and quantum information science. As a physical chemist, I leverage machine learning and AI techniques to solve scientific problems, bridging the gap between experimental and computational research. Passionate about advancing computational science, I seek research and AI/ML related roles in the chemical and materials industries.

SKILLS

Languages and Platforms: Git, SQL, MATLAB, Python, RDKit, PyTorch, TensorFlow, DeepChem

Machine Learning: Linear/Logistic Regression, KNN, Random Forests, Principal Component Analysis, Neural Network

Python Libraries: numpy, pandas, scikit-learn, scipy, matplotlib, seaborn

OS and Platforms: GitHub, Windows, Jupyter Notebook, WSL, Visual Studio Code, Google Colab

Chemistry: accelerator and laser-based science, cheminformatics, kinetic modeling, DFT calculations, FT-IR, X-ray diffraction, mass spectrometry, organic and nanomaterials synthesis, HPLC, NMR, fluorescence, ALD, SEM, TGA

Soft Skills: effective presentation and writing skills, problem-solving, self-starter, working in small teams

SELECTED PROJECTS

DRUG POTENCY PREDICTION ([Project link](#))

- Converted 500+ molecules into graph representation (node and edge structures) using RDKit for deep learning
- Trained 5 different graph neural networks (PyTorch) to predict drug potency from molecular structure (MPNN, GraphSAGE, GCN, GIN, GAT); MPNN and GIN were most effective based on accuracy, recall, and F1 score
- Performed classification and regression tasks to determine drug potency, useful to identify utility of novel molecules

RADICAL ION OPTICAL SPECTRA PREDICTION (ongoing)

- Built chemical database from in-house experimental data and used data reduction techniques to identify patterns in the relationship between molecular structure and optical spectra
- Trained GNNs (PyTorch/PyG) to predict optical spectra and diffusion model to generate molecule candidates
- Validated synthetic feasibility of molecule candidates, both computationally and with experimental domain knowledge

REDOX LADDER OF ENERGY MATERIALS (Brookhaven National Lab)

- Created a new method to measure conjugated polymers for energy applications using accelerator science
- Benchmarked redox levels of state-of-the-art optoelectronic materials (PM6:Y6) for improved materials design
- Used regression analysis to measure materials to millivolt precision in film-like environments, currently unachievable by other methods

PROFESSIONAL EXPERIENCE

BROOKHAVEN NATIONAL LAB (Department of Energy funded research institution)

Postdoctoral Research Associate

Long Island, NY

Sep 2021 – Sep 2025

Joanna Fowler Award in the Chemical Sciences

- Implemented a domain-specific chatbot that employs machine learning and large language models with Python and SQL to accelerate autonomous scientific discovery of materials
- Built a chemical database from scratch with molecular structure and spectral information for deep learning studies
- Applied regression analysis to datasets from laser experiments to calculate the exact energy differences between molecules, generating a new method to measure sustainable materials for solar cells, decreasing the error by 70%
- Constructed magnetic-field dependent experiment at the electron accelerator for molecular quantum information science, making the first observation of quantum beats using electron pulses for room temperature qubits

NORTHWESTERN UNIVERSITY

Doctoral Researcher

Evanston, IL

Aug 2016 – Aug 2021

- Measured kinetics of high-performing, light-responsive organic materials for improved solar cells and photonics using regression and singular value decomposition in MATLAB

- Synthesized novel organic-inorganic hybrid materials via molecular design within nanoporous membranes as photosynthetic mimics, created two new single-cocrystals with different intermolecular stacking geometries
- Designed and managed 5 major projects from end-to-end, collaborating with materials scientists and physicists in cross-functional teams, resulting in 5 peer-reviewed journal publications
- Served as synthesis lab safety officer, mentored 3 graduate students, and designed materials for new chemistry class

LEADERSHIP EXPERIENCE

CHEMISTRY POSTDOC SEMINAR SERIES

Creator and Organizer

Long Island, NY

Sep 2021 – Mar 2023

- Founded the first ever chemistry postdoc seminar series at Brookhaven National Laboratory
- Organized and advertised 30+ seminar presentations and a grad school application panel for SULI summer interns

EDUCATION

NORTHWESTERN UNIVERSITY

Doctor of Philosophy

Physical Chemistry and Materials Science

NSF Graduate Research Fellow

Evanston, IL

Aug 2016 - Aug 2021

COLUMBIA UNIVERSITY

Bachelor of Arts in Chemistry

Société de Chimie Industrielle Fellow

Relevant Coursework: Data Structures and Algorithms in C, Quantum Chemistry, Linear Algebra

New York, NY

Aug 2012 - May 2016

PROFESSIONAL DEVELOPMENT & CERTIFICATIONS

DEEP LEARNING CERTIFICATE

Erdős Institute [project link](#); predicted drug efficacy of small molecules using graph neural networks

May 2025

DATA SCIENCE CERTIFICATE

Erdős Institute [project link](#); automated analysis of NASA chemical data with machine learning

December 2024

RESEARCH SOFTWARE ENGINEERING (INTERSECT PROGRAM)

Princeton University; implementing best software practices (CI/CD, design, code review, testing, packaging)

One of 30 participants selected and fully funded by NSF grant

Princeton, NJ

July 2025

SELECTED PUBLICATIONS

1. **Myong, M. S.**; Bird, M. J.; Miller, J. R. "The Kinetics and Energetics of Electron Transfer to Dimer Radical Cations." *J. Phys. Chem. B*, 2023, 127, 13, 2881-2886
2. **Myong, M. S.**; Qi, Y.; Stern, C. L.; Wasielewski, M. R. "Ultrafast Photo-Driven Charge Transfer Exciton Dynamics in Mixed-Stack Pyrene-Perylenediimide Single Cocrystals." *J. Mater. Chem. C* 2021, 9, 16911-16917
3. **Myong, M. S.**; Young, R. M.; Wasielewski, M. R. "Excimer Diffusivity in 9,10-Bis(phenylethynyl) anthracene Assemblies on Anodic Aluminum Oxide Membranes." *J. Phys. Chem. C* 2021, 125, 44, 24498-24504
4. **Myong, M. S.**; Zhou, J.; Young, R. M.; Wasielewski, M. R. "Charge-Transfer Character in Excimers of Perylenediimides Self-Assembled on Anodic Aluminum Oxide Membranes." *J. Phys. Chem. C* 2020, 124, 8, 4369-4377

SELECTED PRESENTATIONS

1. **Myong, M. S.**; Bird, M. J. "Referenced Redox Potentials of Hole Acceptors in Nonpolar Media" Materials Research Society Spring National Meeting, Seattle, WA, April 2024, oral presentation
2. **Myong, M. S.**; Bird, M. J. "Fundamental Chemical Insights on Molecules and Materials for Sustainable Energy: From Photo- to Electron-Induced Processes." Texas A&M University, Department of Chemistry, December 2023, [invited talk](#).
3. **Myong, M. S.**; Bird, M. J. "Fundamental Chemical Insights on Molecules and Materials for Sustainable Energy: From Photo- to Electron-Induced Processes." University of Texas at Arlington, Department of Chemistry, January 2023, [invited talk](#).
4. **Myong, M. S.**; Bird, M. J. "Fundamental Chemical Insights on Molecules and Materials for Sustainable Energy: From Photo- to Electron-Induced Processes." Baylor University, Department of Chemistry, December 2022, [invited talk](#).