

# Michele Myong, PhD

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

## SUMMARY

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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

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**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

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### 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

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### BROOKHAVEN NATIONAL LAB (Department of Energy funded research institution)

Postdoctoral Research Associate

Joanna Fowler Award in the Chemical Sciences

Long Island, NY

Sep 2021 – Sep 2025

- 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

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### 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

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### NORTHWESTERN UNIVERSITY

Doctor of Philosophy

Evanston, IL

Physical Chemistry and Materials Science

Aug 2016 - Aug 2021

NSF Graduate Research Fellow

### COLUMBIA UNIVERSITY

Bachelor of Arts in Chemistry

New York, NY

Société de Chimie Industrielle Fellow

Aug 2012 - May 2016

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

## PROFESSIONAL DEVELOPMENT & CERTIFICATIONS

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### DEEP LEARNING CERTIFICATE

May 2025

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

### DATA SCIENCE CERTIFICATE

December 2024

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

### RESEARCH SOFTWARE ENGINEERING (INTERSECT PROGRAM)

Princeton, NJ

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

July 2025

One of 30 participants selected and fully funded by NSF grant

## SELECTED PUBLICATIONS

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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

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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](#).