Michele Myong, PhD

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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

AUTOMATED ANALYSIS OF TANDEM MASS SPECTROMETRY (Project link)
- Analyzed a multidimensional dataset from NASA by extracting features with scipy and implementing PCA
- Built KNN and neural networks to automatically correlate features to 10 different minerals in Mars rock
- Accounted for imbalanced data and multi-label classification with Binary Relevance + Random Forest Classifier

PROFESSIONAL EXPERIENCE

BROOKHAVEN NATIONAL LAB (Department of Energy funded research institution) — Long Island, NY
Postdoctoral Research Associate — 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 — Evanston, IL
Doctoral Researcher — 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 Long Island, NY
Creator and Organizer 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 Evanston, IL
Doctor of Philosophy | Advisor: Prof. Michael Wasielewski Aug 2016 - Aug 2021
Physical & Materials Chemistry
NSF Graduate Research Fellow

COLUMBIA UNIVERSITY New York, NY
Bachelor of Arts in Chemistry Aug 2012 - May 2016
Société de Chimie Industrielle Fellow
Relevant Coursework: Data Structures and Algorithms in C, Quantum Chemistry, Linear Algebra

PROFESSIONAL DEVELOPMENT & CERTIFICATIONS

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

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.