

EDUCATION

University of Michigan, Ann Arbor, MI Ph.D. in Chemistry and Scientific Computing	Sep 2018-Mar 2023 GPA: 3.9
Northeastern University, Boston, MA Bachelor of Science in Chemistry and Mathematics	Sep 2014-May 2018 GPA: 4.0

AWARDS AND HONORS

University of Michigan, <i>Rackham One Term Fellowship</i>	Sep 2022-Dec 2022
Michigan Institute for Computational Discovery and Engineering, <i>Fellow</i>	Sep 2018-present
National Science Foundation, <i>Graduate Research Fellowship</i>	Sep 2018-present
Northeastern University, <i>President's Award</i>	Mar 2018
Division of Inorganic Chemistry of the ACS, <i>Undergraduate Award</i>	Aug 2017
Northeastern University, <i>Dean's Scholarship</i>	Sep 2014

SKILLS

Areas of Expertise: quantum chemistry, parallel computing/high performance computing, numerical methods

Proficiencies: Python, C++, MPI+OpenMP, OpenACC, CUDA, CMake, bash, Linux, PyMol, SLURM, BLAS, cuBLAS, PyTorch, TensorFlow (python), scikit-learn, dask, pandas, NumPy, SymPy, Rust, git, Q-Chem, PySCF, Molpro, OpenMolcas, Mathematica

RELEVANT COURSES AND WORKSHOPS

International HPC Summer School, <i>Machine Learning</i>	2022
Nvidia DLI, <i>Fundamentals of Accelerated Data Science</i>	2022
Nvidia DLI, <i>Getting Started with Deep Learning</i>	2022
University of Michigan, <i>Using GPUs with Python</i>	2021
Nvidia DLI, <i>Fundamentals of Accelerated Computing</i>	2020
University of Michigan, <i>Parallel Computing</i>	2019
University of Michigan, <i>Numerical Linear Algebra</i>	2019

EXPERIENCE

Zimmerman Group <i>Graduate Student Researcher</i> , Ann Arbor, MI	May 2019-present
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- Developed a scalable heat-bath CI library in C++ with MPI+OpenMP in the Q-Chem software package.
- Developed incremental CASSCF method for recovering strong correlation in the Q-Chem software package.
- Developed GPU accelerated library for computing Slater integrals with C++ and OpenACC.
- Collaborated with experimental groups to study high-spin organic complexes with significant radicaloid character.
- Collaborated with experimental groups to study photoisomerization processes using DFT and CASSCF.

- University of Michigan** Sep 2019-Apr 2020
Graduate Student Instructor, Ann Arbor, MI
- Led discussions for CHEM 260, an introductory course in Physical Chemistry.
- Geva Group** Jan 2019-May 2019
Graduate Student Researcher (Rotation), Ann Arbor, MI
- Studied applications of the Redfield equation in quantum dynamics simulations and spectroscopy.
- Zimmerman Group** Sep 2018-Dec 2018
Graduate Student Researcher (Rotation), Ann Arbor, MI
- Developed reaction path-finding methods for systematically searching for spin crossings.
- Lopez Lab** Sep 2017-May 2018
Undergraduate Research Assistant, Boston, MA
- Studied photochemical systems, e.g. spiropyrans and diazirines, using DFT and CASSCF in the Gaussian software package.
- Northeastern University** Sep 2017-May 2018
Grader, Boston, MA
- Graded exams and problem sets for Physical Chemistry.
- Pfizer Inc.** Jul 2016-Dec 2016
Co-op Student, Cambridge, MA
- Studied allosteric networks in G-protein coupled receptors with molecular dynamics, docking, and various statistical methods using the Schrödinger, MOE, and Amber software packages.
- Kirss Lab** Dec 2015-May 2018
Undergraduate Research Assistant, Boston, MA
- Studied phosphine exchange and ligand isomerization in $\text{Cp(PPh)}_3\text{RuX}$ complexes using quantum mechanical models in the Gaussian software package.
- Northeastern University** Sep 2015-May 2018
Peer Tutor, Boston, MA
- Tutored students in the Organic and Physical chemistry course series.
- Boeing Co.** May 2015-Aug 2015
Intern - Student Engineer, Huntsville, AL
- Investigated next-generation anodizing and electroplating solutions to replace current methods still utilizing toxic substances.
- Boeing Co.** Jun 2014-Aug 2014
Intern - Student Engineer, Huntington Beach, CA
- Studied adsorption properties of zeolites for CO_2 sequestration.

COMMUNITY INVOLVEMENT

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- American Chemical Society Graduate and Postdoctoral Scholars Office** Apr 2022-Present
Graduate Student Symposium Planning Committee Coordinator, Ann Arbor, MI
- Acted as a liaison between the American Chemical Society's Graduate Student and Postdoctoral Scholar Advisory Board and active Graduate Student Symposium Planning Committees

- Provided logistical support for Graduate Student Symposium Planning Committees at American Chemical Society National Meetings

University of Michigan Graduate Student Symposium Planning Committee **Nov 2018-Nov 2020**
American Chemical Society Correspondent, Ann Arbor, MI

- Planned the Graduate Student Symposium for the American Chemical Society National Meeting in Philadelphia 2020.

Northeastern University Student Affiliates of the ACS **May 2017-May 2018**
President, Boston, MA

- Acted as a bridge between the undergraduate chemistry students and the chemistry department.
- Hosted weekly speakers to discuss current research and future career opportunities for chemistry graduates.

Northeastern University College of Science Advisory Council **Sep 2015-May 2018**
Chemistry Representative, Boston, MA

- Advised the deans of the College of Science on important issues of the undergraduate student body.

Northeastern University Student Affiliates of the ACS **May 2016-May 2017**
Secretary, Boston, MA

- Wrote a semi-weekly newsletter about upcoming events and opportunities to the chemistry undergraduates.
- Invited professionals in chemistry to discuss relevant research and career opportunities to participate in the club’s weekly speaker series.

Beyond Benign **Oct 2015-May 2018**
Green Chemistry Outreach Fellow, Wilmington, MA

- Participated in outreach events to promote the principles of green chemistry and engage young students in science.

PUBLICATIONS

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9. **D.-K. Dang**, J.D. Einkauf, X. Ma, Y. Ma, B.A. Moyer, P.M. Zimmerman, V.S. Bryantsev, Computational and Spectroscopic Characterization of the Photoresponsive 2-Pyridylaminoguanidinium Ligand, *manuscript in preparation*.
 8. B. Prajapati, M. Ambhore, **D.-K. Dang**, P. Chmielewski, T. Lis, C. Gómez-García, P.M. Zimmerman, M. Stepień, Tetrafluorenofulvalene: A Sterically Frustrated Open-Shell Alkene, *Nature Chemistry*, *manuscript in review*.
 7. S. Tribedi, **D.-K. Dang**, B. Kanungo, V. Gavini, P.M. Zimmerman, Exchange Correlation Potentials from Accurate FCI Densities Constructed from Slater Basis Functions, arXiv:2302.11999 [physics.chem-ph]
 6. **D.-K. Dang**, J. A. Kammeraad, P. M. Zimmerman, Advances in Parallel Heat Bath Configuration Interaction, *J. Phys. Chem. A*, 2023, **127**(1), 400.
 5. **D.-K. Dang**, L. W. Wilson, P. M. Zimmerman, The numerical evaluation of Slater integrals on graphics processing units, *J. Comput. Chem.*, 2022, **43**(25), 1680.
 4. B. Prajapati, **D.-K. Dang**, P. J. Chmielewski, M. A. Majewski, T. Lis, C. J. Gómez-García, P. M. Zimmerman, M. Stepień, An Open-Shell Coronoid with Hybrid Chichibabin–Schlenk Conjugation, *Angew. Chem. Int. Ed.* 2021, **60**, 22496.
 3. **D.-K. Dang** and P. M. Zimmerman, Fully Variational Incremental CASSCF, *J. Chem. Phys.*, 2021, **154**, 014105

2. V. M. Breslin, N. A. Barbour, **D.-K. Dang**, S. A. Lopez, and M. A. Garcia-Garibay, Nanosecond laser flash photolysis of a 6-nitroindolinospiropyran in solution and in nanocrystalline suspension under single excitation conditions, *Photochem. Photobiol. Sci.*, 2018, **17**, 741
1. D. Hill, C. Delaney, M. Clark, M. Eaton, B. Hassan, O. Hendricks, **D.-K. Dang**, and R.U. Kirss, Kinetics of phosphine substitution in $\text{CpRu}(\text{PPh}_3)_2\text{X}$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}, \text{N}_3$, and NCO), *RSC Adv.*, 2017, **7**, 34425

PRESENTATIONS

6. **D.-K. Dang**, P. M. Zimmerman, Advances in Parallel Heat-Bath Configuration Interaction, Michigan Institute for Computational Discovery and Engineering Symposium, March 24, (2023)
5. **D.-K. Dang**, L. W. Wilson, P. M. Zimmerman, GPU-accelerated numerical integration of electron repulsion integrals in a Slater basis, ACS Spring National Meeting & Events, San Diego, CA, United States, March 20-24, (2022), COMP
4. **D.-K. Dang**, P. M. Zimmerman, Treating Large CASSCF Active Spaces with the Method of Increments, 33rd Annual Workshop on Recent Developments in Electronic Structure Methods (ES21), (2021)
3. **D.-K. Dang**, P. M. Zimmerman, Variational procedure for the many-body expansion of the CASSCF energy, 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, (2020), COMP-0591
2. M. C. Enright, A. Giarross, J. Romeo, **D.-K. Dang**, J. Davis, C. Olbrich. Empowering undergraduates to be green chemistry ambassadors in their community through outreach, 21st Annual Green Chemistry & Engineering Conference, Reston, VA, United States, June 13-15 (2017), GC+E-239
1. **D.-K. Dang**, and R. U. Kirss. Linkage isomerization in phosphine substitution reactions of $\text{CpRu}(\text{PPh}_3)_2\text{NCS}$, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, (2017), COMP-323.