930 N. University Ave
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Duy-Khoi Dang

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EDUCATION

University of Michigan, Ann Arbor, MI — **Sep 2018-Mar 2023**
Ph.D. in Chemistry and Scientific Computing — GPA: 3.9

Northeastern University, Boston, MA — **Sep 2014-May 2018**
Bachelor of Science in Chemistry and Mathematics — GPA: 4.0

AWARDS AND HONORS

University of Michigan, *Rackham One Term Fellowship* — **Sep 2022-Dec 2022**

Michigan Institute for Computational Discovery and Engineering, *Fellow* — **Sep 2018-present**

National Science Foundation, *Graduate Research Fellowship* — **Sep 2018-present**

Northeastern University, *President's Award* — **Mar 2018**

Division of Inorganic Chemistry of the ACS, *Undergraduate Award* — **Aug 2017**

Northeastern University, *Dean's Scholarship* — **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, *Machine Learning* — **2022**

Nvidia DLI, *Fundamentals of Accelerated Data Science* — **2022**

Nvidia DLI, *Getting Started with Deep Learning* — **2022**

University of Michigan, *Using GPUs with Python* — **2021**

Nvidia DLI, *Fundamentals of Accelerated Computing* — **2020**

University of Michigan, *Parallel Computing* — **2019**

University of Michigan, *Numerical Linear Algebra* — **2019**

EXPERIENCE

TSMC
Principal Engineer, San Jose, CA — **Jul 2023-Present**

Zimmerman Group
Graduate Student Research Assistant, Ann Arbor, MI — **May 2019-Mar 2023**
Postdoctoral Researcher, Ann Arbor, MI — **Mar 2023-Jun 2023**

- 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
Graduate Student Instructor, Ann Arbor, MI **Sep 2019-Apr 2020**

- Led discussions for CHEM 260, an introductory course in Physical Chemistry.

Geva Group
Rotation Student, Ann Arbor, MI **Jan 2019-May 2019**

- Studied applications of the Redfield equation in quantum dynamics simulations and spectroscopy.

Zimmerman Group
Rotation Student, Ann Arbor, MI **Sep 2018-Dec 2018**

- Developed reaction path-finding methods for systematically searching for spin crossings.

Lopez Lab
Undergraduate Research Assistant, Boston, MA **Sep 2017-May 2018**

- Studied photochemical systems, e.g. spiropyrans and diazirines, using DFT and CASSCF in the Gaussian software package.

Northeastern University
Grader, Boston, MA **Sep 2017-May 2018**

- Graded exams and problem sets for Physical Chemistry.

Pfizer Inc.
Co-op Student, Cambridge, MA **Jul 2016-Dec 2016**

- 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
Undergraduate Research Assistant, Boston, MA **Dec 2015-May 2018**

- Studied phosphine exchange and ligand isomerization in $Cp(PPh)_3RuX$ complexes using quantum mechanical models in the Gaussian software package.

Northeastern University
Peer Tutor, Boston, MA **Sep 2015-May 2018**

- Tutored students in the Organic and Physical chemistry course series.

Boeing Co.
Intern - Student Engineer, Huntsville, AL **May 2015-Aug 2015**

- Investigated next-generation anodizing and electroplating solutions to replace current methods still utilizing toxic substances.

Boeing Co.
Intern - Student Engineer, Huntington Beach, CA **Jun 2014-Aug 2014**

- Studied adsorption properties of zeolites for CO_2 sequestration.

COMMUNITY INVOLVEMENT

American Chemical Society Graduate and Postdoctoral Scholars Office
Graduate Student Symposium Planning Committee Coordinator, Ann Arbor, MI   **Apr 2022-Present**

- Acted as a liason 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
American Chemical Society Correspondent, Ann Arbor, MI   **Nov 2018-Nov 2020**

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

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

- 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
Chemistry Representative, Boston, MA   **Sep 2015-May 2018**

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

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

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

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

PUBLICATIONS

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. Stępień, 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. Stępień, 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 $CpRu(PPh_3)_2X$ (X = Cl, Br, I, 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 Institue 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 $CpRu(PPh_3)_2NCS$, 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, (2017), COMP-323.