Duy-Khoi Dang

San Jose, CA | khoidang@umich.edu | khoidang.com
github.com/duykhoidang | ORCID: 0000-0001-7530-0540

Education

University of Michigan, Ann Arbor, MI — Sep 2018 - Apr 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
NSF XSEDE, *Startup Allocation on SDSC Expanse* — May 2022 - May 2023
Michigan Institute for Computation Discovery and Engineering, *Fellow* — Sep 2018 - Apr 2023
National Science Foundation, *Graduate Research Fellowship* — Sep 2018 - Apr 2023
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 - May 2018

Skills

Areas of Expertise: quantum chemistry, parallel computing, high performance computing

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

Experience

TSMC
Principal Engineer, San Jose, CA — Jul 2023 - Present
- Contributed to and maintained scientific software library for lithography simulations using CUDA and C++
- Developed in-house machine-learning inferencing engines in CUDA and C++ to obtain speedup over TensorFlow
- Developed high-performance polygon algorithms and engines for CPU and GPU

Zimmerman Group
Graduate Student Research Assistant, Ann Arbor, MI — May 2019 - Apr 2023
- Developed scalable heat-bath CI library in C++ with MPI+OpenMP in Q-Chem software package
- Devloped incremental CASSCF methods for recovering strong correlation in 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 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 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, specifically 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 statistical methods using using the Schödinger, 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 DFT in the Gaussian software package

Northeastern University
Peer Tutor, Boston, MA Sep 2015 - May 2018
- Tutored students in 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 incumbent methods utilizing toxic substances

Boeing Co.
Intern - Student Engineer, Huntington Beach, CA Jun 2014 - Aug 2014
- Studied CO_2 adsorption properties of zeolites

Community Involvement

American Chemical Society Graduate and Postdoctoral Scholars Office
Graduate Student Symposium Planning Committee Coordinator Apr 2022 - Sep 2024
- 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 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 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 throughout the Boston Area to promote the principles of green chemistry and engage young students in science

Publications

12. Y.-Z. Ma, J. D. Einkauf, X. Ma, **D.-K. Dang**, P. M. Zimmerman, R. Custelcean, B. Doughty, V. S. Bryantsev, Photoswitching dynamics of a guanidine anion receptor, *Phys. Chem. Chem. Phys.*, 2025, **27**, 13434-13446.

11. J. Hatch, A. E. Rask, **D.-K. Dang**, P. M. Zimmerman, Many-Body Basis Set Amelioration Method for Incremental Full Configuration Interaction, *J. Phys. Chem. A*, 2025, **129**, 3743-3753.

10. **D.-K. Dang**, J. D. Einkauf, X. Ma, R. Custelcean, Y.-Z. Ma, P. M. Zimmerman, V. S. Bryantsev, Photoisomerization mechanism of iminoguanidinium receptors from spectroscopic methods and quantum chemical calculations, *Phys. Chem. Chem. Phys.*, 2024, **26**, 24008-24020.

9. 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, *Nat. Chem.*, 2023, **15**, 1541.

8. **D.-K. Dang**, D. Cehreli, B. S. Rich, T. E. Haas, F. R. Fronczek, and R. U. Kirss, Phosphine substitution and linkage isomerization in cyclopentadienylruthenium bis(triphenylphosphine)thiocyanide and selenocyanide, $CpRu(PPh_3)_2NCS$ and $CpRu(PPh_3)_2SeCN$, *Dalton Trans.*, 2023, **52**, 13258.

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, *J. Chem. Phys.* 2023, **159**, 054106.

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.