

Claire E. Dickerson

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EDUCATION

Ph.D., Theoretical Chemistry: **University of California, Los Angeles** September 2019 – Present
Advisor: Prof. Anastassia Alexandrova (Los Angeles, CA)

B.S., Chemistry: **University of Rochester** August 2014 – May 2018
Advisor: Prof. Kara Bren (Rochester, NY)

SKILLS

- Proficient in Python, C++, Bash and working in a Unix Environment
- Quantum chemistry software (Gaussian, Molcas, Molpro, Q-Chem, SHCI, Turbomole, VASP)

EXPERIENCE

UCLA: Graduate Student Researcher September 2019 – Present
Supervisor: Prof. Anastassia Alexandrova (Los Angeles, CA)

- Electronic structure theory and molecular qubits

HRL Laboratories: Doctorate Intern June 2021 – September 2021
Supervisor: Dr. Andrew Pan (Malibu, CA)

- Applied and extended configuration interaction methods for quantum dot spin qubits
- Worked on techniques for more efficient calculation and description of quantum dot wave functions

Schrödinger: Jaguar Intern June 2019 – September 2019
Supervisor: Dr. Art Bochevarov (New York, NY)

- Developed workflow using quantum mechanical methods for automated ring-chain tautomer generation without rules

University of Sydney, Quantum Control Laboratory: Visiting Researcher July 2018 – June 2019
Supervisors: Profs. Ivan Kassal and Michael Biercuk (Sydney, AU)

- Developed new computational tools in Mathematica for simulating quantum phenomena on a trapped-ion quantum computer

University of Rochester: Research Assistant May 2016 – June 2018
Supervisors: Prof. Kara Bren (Rochester, NY)

- Characterized and evaluated catalytic efficiency of metallopeptides which evolve hydrogen and reduce nitrite from water, functionally mimicking Cytochrome c
- Used *ab initio* dynamics to elucidate coordination structure of a catalyst, which could not be crystallized, for each step in a proposed reaction mechanism and its transition states

NASA Ames: Quantum Chemistry Intern June 2017 – September 2017
Supervisors: Drs. Timothy Lee and Partha Bera (Mountain View, CA)

- Used *ab initio* methods to characterize prebiotic molecules in the interstellar medium by identifying transition states, relative energies and optimized geometries

AWARDS

NSF Graduate Research Fellowship March 2021

UCLA CQSE Fellowship (Center for Quantum Science and Engineering) October 2020

COMP Division Workshop & Career Roundtable (ACS) March 2018

BAER Institute Scholarship (Bay Area Environmental Research Institute) September 2017

PUBLICATIONS

1. Optical Cycling Functionalization of Arenes. **C.E. Dickerson**, H. Guo, G. Guozhu, J. Caram, E. Hudson, W. Campbell, A. Alexandrova. *J. Phys. Chem. Lett.* **2021**, *12* (16), 3989-3995.
2. Analog quantum simulation of chemical dynamics. R.J. MacDonnell, **C.E. Dickerson**, C. Birch, A. Kumar, C. Edmunds, M.J. Biercuk, C. Hempel and I. Kassal. *Chem. Sci.* **2021**, *12*, 9794-9805.
3. Franck-Condon tuning of optical cycling centers by organic functionalization. **C.E. Dickerson***, H. Guo*, J. Caram, W. Campbell, A.J. Shin, B.L. Augenbraun and A. Alexandrova. *Phys. Rev. Lett.* **2021**, *126* (12), 123002.
4. Surface Chemical Trapping of Optical Cycling Centers. H. Guo, **C.E. Dickerson**, A.J. Shin, C. Zhao, T. Atallah, J. Caram, W. Campbell and A. Alexandrova. *Phys. Chem. Chem. Phys.* **2021**, *21* (1), 211-218.
5. Pattern-free generation and quantum-mechanical scoring of ring-chain tautomers. D.S. Levine, M.A. Watson, L.D. Jacobson, **C.E. Dickerson**, H.S. Yu and A.D. Bochevarov. *J. Comput. Aided Mol. Des.* **2020**, 1-15.
6. Characterization of Azirine and Its Structural Isomers. **C.E. Dickerson**, P.P. Bera and T.J. Lee. *J. Phys. Chem. A.* **2018**, *122*, 8898-8904.
7. A Cobalt Metallopeptide Electrocatalyst for the Selective Reduction of Nitrite to Ammonium. Y. Guo, J.R. Stroka, B. Kandemir, **C.E. Dickerson**, and K.L. Bren. *J. Am. Chem. Soc.* **2018**, *140*, 16888-169.

*Authors contributed equally.