

Frank Hovorka Assistant Professor of Chemistry
Case Western Reserve University
Department of Chemistry
10900 Euclid Ave., Cleveland, OH 44106

web: quantumparker.com
ph: (216) 368-3697
orcid: 0000-0002-1110-3393
scholar: OqC2Vc8AAAAJ

positions

2021 –	Frank Hovorka Assistant Professor of Chemistry Case Western Reserve University	Cleveland, OH
2019 – 2021	Assistant Professor of Chemistry Case Western Reserve University	Cleveland, OH
2014 – 2019	Postdoctoral Fellow (as Arnold O. Beckman Postdoctoral Fellow 2016 -- 2019) University of California Irvine <i>Advisor:</i> Professor Filipp Furche	Irvine, CA
2009 – 2014	PhD, Theoretical Chemistry Northwestern University <i>Advisor:</i> Professor Mark Ratner and Professor Tamar Seideman	Evanston, IL
2008 – 2009	Fulbright Fellow Technische Universität München <i>Advisor:</i> Professor Notker Rösch	Munich, Germany
2004 – 2008	B.S., Chemistry & B.S., Mathematics University of Florida <i>Advisor:</i> Professor N. Yngve Öhrn	Gainesville, FL

professional affiliations

- Member of the American Chemical Society
- Member of the American Physical Society

awards

2021	Finalist, John S. Diekhoff Award for Distinguished Graduate Student Teaching, CWRU
2021 – 2024	Frank Hovorka Assistant Professor of Chemistry, CWRU
2020 – 2021	Glennan Fellowship, CWRU Pedagogical Award
2020	STAIR Mentor Fellows Program, CWRU
2019	Nominated, John S. Diekhoff Award for Distinguished Graduate Student Teaching, CWRU
2016 – 2019	Arnold O. Beckman Postdoctoral Fellowship
2010 – 2013	Department of Energy Office of Science Graduate Fellowship
2009	Participant, 59th Lindau Nobel Laureate Meeting
2008 – 2009	Fulbright Fellowship Technische Universität München
2006	Anderson Scholar with Highest Distinction, UF academic achievement and uninterrupted study

publications

 corresponding authorship denoted with *

Case Western Reserve University

- E. Roy Miller, [S. M. Parker*](#),
Numerically Stable Resonating Hartree-Fock, **2024**, submitted, arXiv:2411.00712
- 26 W. B. Martin, R. E. Warburton, [S. M. Parker](#), V. O. Rodionov,
On the characterization of γ -graphyne, *Nature Synthesis* **2024**, doi: 10.1038/s44160-024-00642-1, chemRxiv:2023.xl3gp.v3
- 25 Z. Zhou, [S. M. Parker*](#),
Converging TDDFT calculations in 5 iterations with minimal auxiliary preconditioning, *Journal of Chemical Theory and Computation* **2024**, 20, 6738-6746, doi: 10.1021/acs.jctc.4c00577, arXiv:2404.17133

- 24 E. Roy Miller, S. J. Hoehn, A. Kumar, D. Jiang, S. M. Parker*,
Ultrafast Photochemistry and Electron Diffraction for Cyclobutanone in the S₂ State: Surface Hopping with Time-Dependent Density Functional Theory, *The Journal of Chemical Physics* **2024**, *161*, 034105, doi: 10.1063/5.0203679, arXiv:2402.10336
- 23 Y. J. Franzke, C. Holzer, J. H. Andersen, T. Begusic, F. Bruder, S. Coriani, F. Della Sala, E. Fabiano, D. A. Fedotov, S. Fürst, S. Gillhuber, R. Grotjahn, M. Kaupp, M. Kehry, M. Krstic, F. Mack, S. Majumdar, B. D. Nguyen, S. M. Parker, F. Pauly, A. Pausch, E. Perlt, G. S. Phun, A. Rajabi, D. Rappoport, B. Samal, T. Schrader, M. Sharma, E. Tapavicza, R. S. Treß, V. Voora, A. Wodynski, J. M. Yu, B. Zerulla, F. Furche, C. Hättig, M. Sierka, D. P. Tew, F. Weigend,
Turbomole: Today and Tomorrow, *Journal of Chemical Theory and Computation* **2023**, *19*, 6859-6890, doi: 10.1021/acs.jctc.3c00000
- 22 Z. Zhou, F. Della Sala, S. M. Parker*,
Minimal auxiliary basis set approach for the electronic excitation spectra of organic molecules, *The Journal of Physical Chemistry Letters* **2023**, *14*, 1968-1976, doi: 10.1021/acs.jpclett.2c03698, submitted version
- 21 V. G. Desyatkin, W. B. Martin, A. E. Aliev, N. E. Chapman, A. F. Fonseca, D. S. Galvão, E. Roy Miller, K. H. Stone, Z. Wang, D. Zakhidov, F. T. Limpoco, S. R. Almahdali, S. M. Parker, R. H. Baughman, V. O. Rodionov,
Scalable Synthesis and Characterization of Multilayer γ -Graphyne, New Carbon Crystals with a Small Direct Band Gap, *Journal of the American Chemical Society* **2022**, *144*, 17999-18008, doi: 10.1021/jacs.2c06583, arXiv:2301.05291
- 20 Z. Zhou, S. M. Parker*,
Accelerating molecular property calculations with semiempirical preconditioning, *The Journal of Chemical Physics* **2021**, *155*, 204111, doi: 10.1063/5.0071013, accepted version
- 19 M. Gupta, M. Singha, D. Rasale, Z. Zhou, S. Bhandari, S. Beasley, J. Sakr, S. M. Parker, R. Spitale,
Mutually orthogonal bioconjugation of vinyl nucleosides for RNA metabolic labeling, *Organic Letters* **2021**, *23*, 7183-7187, doi: 10.1021/acs.orglett.1c02584
- 18 J. Jimenez, Z. Zhou, A. L. Rheingold, S. M. Parker, G. Sauvé,
Tuning the properties of azadipyrromethene-based near-infrared dyes using intramolecular BO-chelation and peripheral substitutions, *Inorganic Chemistry* **2021**, *60*, 13320-13331, doi: 10.1021/acs.inorgchem.1c01597
- 17 S. M. Parker*, C. J. Schiltz,
Surface hopping with cumulative probabilities: even sampling and improved reproducibility, *The Journal of Chemical Physics* **2020**, *153*, 174109, doi: 10.1063/5.0024372, accepted version

Before Case Western Reserve University

- 16 S. Balasubramani, G. P. Chen, S. Coriani, M. Diedenhofen, M. S. Frank, Y. J. Franzke, F. Furche, R. Grotjahn, M. E. Harding, C. Hättig, A. Hellweg, B. Helmich-Paris, C. Holzer, U. Huniar, M. Kaupp, A. Marefat Khah, S. Karbalaei Khani, T. Müller, F. Mack, B. D. Nguyen, S. M. Parker, E. Perlt, D. Rappoport, K. Reiter, S. Roy, M. Rückert, G. Schmitz, M. Sierka, E. Tapavicza, D. P. Tew, C. van Wüllen, V. K. Voora, F. Weigend, A. Wodyński, J. M. Yu,
TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations, *The Journal of Chemical Physics* **2020**, *152*, 184107, doi: 10.1063/5.0004635
- 15 S. M. Parker, S. Roy, F. Furche,
Multistate hybrid time-dependent density functional theory with surface hopping accurately captures ultrafast thymine photodeactivation, *Physical Chemistry Chemical Physics* **2019**, *21*, 18999-19010, doi: 10.1039/C9CP03127H
- 14 M. Kubota, S. Nainar, S. M. Parker, W. England, F. Furche, R. Spitale,
Expanding the Scope of RNA Metabolic Labeling with Vinyl Nucleosides and Inverse Electron-Demand Diels-Alder Chemistry, *ACS Chemical Biology* **2019**, *14*, 1698-1707, doi: 10.1021/acschembio.9b00079
- 13 S. M. Parker, D. Rappoport, F. Furche,
Quadratic response properties from TDDFT: trials and tribulations, *Journal of Chemical Theory and Computation* **2018**, *14*, 807-819, doi: 10.1021/acs.jctc.7b01008
- 12 M. Muuronen, S. M. Parker, E. Berardo, A. Le, M. Zwijnenburg, F. Furche,
Mechanism of Photocatalytic Water Oxidation on Small TiO₂ Nanoparticles, *Chemical Science* **2017**, *8*, 2179-2183, doi: 10.1039/C6SC04378J

- 11 S. M. Parker, S. Roy, and F. Furche,
Unphysical divergences in response theory, *The Journal of Chemical Physics* **2016**, *145*, 134105, doi: 10.1063/1.4963749
- 10 V. A. Nasluzov, S. M. Parker, A. Genest, A. M. Shor, E. A. Ivanova-Shor, N. Rösch,
Trinuclear tantalum clusters grafted to hydroxylated silica surfaces: A density-functional embedded-cluster study, *Kinetics and Catalysis* **2015**, *56*, 631, doi: 10.1134/S0023158415050134
- 9 I. Kim, S. M. Parker, T. Shiozaki,
Orbital Optimization in the Active Space Decomposition Model, *Journal of Chemical Theory and Computation* **2015**, *11*, 3636, doi: 10.1021/acs.jctc.5b00429, arXiv:1505.02346
- 8 S. M. Parker, T. Shiozaki,
Active space Decomposition with multiple sites: Density matrix renormalization group algorithm, *The Journal of Chemical Physics* **2014**, *141*, 211102, doi: 10.1063/1.4902991, arXiv:1410.6407
- 7 S. M. Parker, M. Smeu, I. Franco, M. A. Ratner, T. Seideman,
Molecular Junctions: Can Pulling Influence Optical Controllability, *Nano Letters* **2014**, *14*, 4587, doi: 10.1021/nl501629c
- 6 S. M. Parker, T. Shiozaki,
Quasi-diabatic states from active space decomposition, *Journal of Chemical Theory and Computation* **2014**, *10*, 3738, doi: 10.1021/ct5004753
- 5 S. M. Parker*, T. Seideman, M. A. Ratner, T. Shiozaki,
Model Hamiltonian analysis of singlet fission from first principles, *Journal of Physical Chemistry C* **2014**, *118*, 12700, doi: 10.1021/jp505082a
- 4 S. M. Parker*, T. Seideman, M. A. Ratner, T. Shiozaki,
Active-space decomposition for molecular dimers, *The Journal of Chemical Physics* **2013**, *139*, 021108, doi: 10.1063/1.4813827
- 3 Y. Wu, V. A. Karttunen, S. M. Parker, A. Genest, N. Rösch,
Olefin Hydrosilylation Catalyzed by a Bis-N-Heterocyclic Carbene Rhodium Complex. A Density Functional Theory Study, *Organometallics* **2013**, *32*, 2363, doi: 10.1021/om301236n
- 2 S. M. Parker, M. A. Ratner, T. Seideman,
Simulating strong field control of axial chirality using optimal control theory, *Molecular Physics* **2012**, *110*, 1941, doi: 10.1080/00268976.2012.695808
- 1 S. M. Parker, M. A. Ratner, T. Seideman,
Coherent control of molecular torsion, *The Journal of Chemical Physics* **2011**, *135*, 224301, doi: 10.1063/1.3663710

book chapters

Before Case Western Reserve University

- 1 S. M. Parker, F. Furche
Frontiers in Quantum Chemistry, edited by M. J. Wójcik, H. Nakatsuji, B. Kirtman, Y. Ozaki, Springer Singapore (2018)
Response theory and molecular properties

reports in media and professional journals

2020	Scilight featured article	Photochemistry simulations dramatically improve reliability and reproducibility
2020	JCP Editor's choice	Cumulative surface hopping paper highlighted by AIP
2019	CCPC Editor's choice	Multi-state TDDFT paper selected as outstanding article by Editor-in-Chief

talks

Case Western Reserve University

September 18, 2024	TDDFT-ris: A semiempirical model and preconditioner for fast and accurate spectra and nonlinear properties (invited) Turbomole User and Developer Meeting	Oxford, UK
July 10, 2024	TDDFT-ris: A semiempirical model and preconditioner for fast and accurate spectra and nonlinear properties (invited) CECAM Reaction Prediction Workshop	Chicago, IL
June 7, 2024	Towards Photochemistry with the Resonating Mean-Field Method (invited) ACS Mid-Atlantic Regional Meeting	State College, PA
May 31, 2024	Towards Photochemistry with the Resonating Mean-Field Method (invited) Madison, WI Midwest Theoretical Chemistry Conference 2024	University of Wisconsin-Madison,
March 17-18, 2024	(1) TDDFT-ris: A semiempirical model and preconditioner for fast and accurate spectra (2) Hop to it: cumulative probabilities make surface hopping simulations cheaper and more reproducible Meeting of the American Chemical Society	New Orleans, LA
January 16, 2024	Simulating Photochemistry from First-Principles Quantum Chemistry (invited) University of Akron	Akron, OH
September 11, 2023	Computational Photochemistry (invited) Binghamton University, Department of Physics	Binghamton, NY
July 6, 2023	Fast spectra with the minimal auxiliary basis approach to TDDFT (invited) Rutgers TDDFT Workshop	Rutgers, NJ
June 3, 2023	Fast spectra with the minimal auxiliary basis approach to TDDFT Midwest Theoretical Chemistry Conference 2023	Purdue University, West Lafayette, IN
October 2022	Fast Spectra with the minimal auxiliary basis approach to TDDFT (invited) Benasque 9th TDDFT Workshop	Benasque, Spain
August 2022	Accelerating Quantum Chemistry with Semiempirical Preconditioning (invited) CWRU-Tohoku 8th Annual Data Science in Engineering and Life Sciences Symposium	Cleveland, Ohio
June 2022	Accelerating TDDFT with Semiempirical Preconditioning 52nd MWTCC	Columbus, Ohio
March 2022	Cumulative Surface Hopping: Faster and More Reproducible APS March Meeting 2022	Chicago, Illinois

Before Case Western Reserve University

August 2018	Excited-State Chemistry with TDDFT (invited) 256th American Chemical Society National Meeting and Exposition	Boston, Massachusetts
August 2018	Ensemble Optimized Time-Dependent Density Functional Theory (invited) 256th American Chemical Society National Meeting and Exposition	Boston, Massachusetts
March 2018	Quadratic response properties from TDDFT: trials and tribulations APS March Meeting	Los Angeles, California
July 2017	Nonlinear properties from TDDFT: trials and tribulations (invited) Excited States: Electronic Structure and Dynamics	Telluride, Colorado
April 2017	Nonlinear properties from TDDFT: trials and tribulations (invited) 253rd American Chemical Society National Meeting and Exposition	San Francisco, California
March 2016	Diagnosis and implications of spurious poles in the quadratic response of approximate electronic structure methods 251st American Chemical Society National Meeting and Exposition	San Diego, California
June 2015	Non-adiabatic molecular dynamics (invited) 98th Meeting of the Canadian Society of Chemistry	Ottawa, Ontario
June 2014	Model Hamiltonians from the Active-space Decomposition Method (invited) McMaster University, Department of Chemistry	Hamilton, Ontario

pedagogical lectures

Case Western Reserve University

October 2022 **TDDFT in Chemistry and Biochemistry (2 lectures)**
Benasque 9th TDDFT School

Benasque, Spain

Before Case Western Reserve University

July 2017 **Nonadiabatic molecular dynamics with TDDFT (2 lectures)**
Telluride School on Time-dependent Density Functional Theory

Telluride, Colorado

support

funded support

- **Project Title:** Photochemistry with Resonating Mean-Field
Amount: \$650,000 (100% Parker)
Role: PI
Source: NSF CAREER, Division of Chemistry (CHE)
Status: current
Start Date: 06/01/2023 **End Date:** 05/30/2028
Award ID: CHE-2236959
- **Project Title:** Chemistry on Computers at CWRU
Amount: \$6,500
Role: PI
Source: Case Western Reserve University
Status: completed
Start Date: 07/2020 **End Date:** 06/2021

pending support

- **Project Title:** Exploratory Optoelectronic Characterization and Simulation of Graphyne
Amount: \$40,000 (45% Parker)
Role: PI (co-PIs: Clemens Burda, Valentin Rodionov)
Source: Case Western Reserve University
Status: pending
- **Project Title:** Spatial and Temporal Control of Energy Transfer at the Atomic Scale in DNA Photonic Materials
Amount: \$40,000 (33% Parker)
Role: co-PI (PI: Carlos Crespo, co-PI: Divita Mathur)
Source: Case Western Reserve University
Status: pending

declined support

- **Project Title:** FuSe_2 : Carbon Semiconductor Devices Based on γ -Graphyne
Amount: \$2,000,000 (17% Parker)
Role: co-PI (PI: Valentin Rodionov)
Source: NSF Future of Semiconductors (FuSe_2)
Status: declined
- **Project Title:** Early Career: A Multiscale Approach to Simulating Photochemistry in Complex Environments
Role: PI
Source: Department of Energy
Status: preproposal discouraged
- **Project Title:** Fast nonlinear properties calculations for predicted transient spectra through a minimal-auxiliary basis set method
Amount: \$100,000
Role: PI
Source: Camille Dreyfus Teacher-Scholar Awards Program
Status: declined
- **Project Title:** Computing Nonlinear Optical Phenomena at All Orders Through the Action Lagrangian Eigenvalue Problem
Amount: \$120,000
Role: PI

Source: Cottrell Scholar Award - Research Corporation for Science Advancement

Status: declined

- **Project Title:** FuSe: Carbon Semiconductor Devices Based on γ -Graphyne
Amount: \$2,000,000 (20% Parker)
Role: co-PI (PI: Valentin Rodionov)
Source: NSF Future of Semiconductors (FuSe)
Status: declined
- **Project Title:** Controlling the Donor and Acceptor Distance, Orientation, and Motions in Donor-Acceptor DNA Biophotonic Materials to Optimize their Energy Transfer Efficiencies
Amount: \$2,000,000 (33% Parker)
Role: PI
Source: NSF DMREF
Status: declined
- **Project Title:** Early Career: Enabling First-Principles Solar Fuel Simulations by Accelerating Photochemistry Simulations
Amount: \$875,000
Role: PI
Source: Department of Energy
Status: preproposal discouraged
- **Project Title:** EFRC: Center for Reactivity and Dynamics at Electrocatalytic Interfaces
Role: co-PI (PI: Daniel Scherson)
Source: Department of Energy
Status: white paper discouraged
- **Project Title:** Driver-assistance for Quantum Chemistry
Amount: \$120,000
Role: PI
Source: Dreyfus Program for Machine Learning in The Chemical Sciences and Engineering
Status: declined
- **Project Title:** First-principles computational photochemistry
Amount: \$250,000
Role: PI
Source: 2023 Blavatnik National Awards for Young Scientists
Status: declined
- **Project Title:** Early Career: Accelerating Photochemistry Simulations with Cumulative Sampling
Amount: \$750,000
Role: PI
Source: Department of Energy
Status: declined
- **Project Title:** Synthetic pathways to γ -graphyne and related allotropes of carbon
Amount: \$1,000,000 (50% Parker)
Role: co-PI (PI: Valentin Rodionov)
Source: W.M. Keck Foundation
Status: declined
- **Project Title:** Decomposition of Complex Macromolecular Architectures Under External Stressors: Computation, Spectroscopy, and Graph-Neural-Network Learning
Amount: \$7,500,000 (15% Parker)
Role: co-PI (PI: Prof. Roger French)
Source: Department of Defense - MURI
Status: white paper discouraged

student fellowships

- **student:** Ericka Miller
title: Implementing an efficient, stable, and open-source version of the state-averaged Resonating Hartree-Fock method for use in photochemical applications
fellowship: Molecular Sciences Software Fellowship

amount: \$53,092

dates – 07/01/2023 – 06/30/2024

collaborators

Case Western Reserve University

- Prof. Genevieve Sauve (CWRU Chemistry)
- Prof. Valentin Rodionov (CWRU Chemistry)
- Prof. Clemens Burda (CWRU Chemistry)
- Prof. Carlos Crespo (CWRU Chemistry)
- Prof. Divita Mathur (CWRU Chemistry)
- Prof. Matthew Bertin (CWRU Chemistry)
- Prof. Metin Karayilan (CWRU Chemistry)

External

- Prof. Robert Spitale (University of California, Irvine — Department of Chemistry)
- Prof. Fabio Della Sala (Center for Biomolecular Nanotechnologies, Istituto Italiano di Tecnologia; Institute for Microelectronics and Microsystems (CNR-IMM))

service

- Member, Faculty Search Committee (AY2023-24)
- Member, Artificial Intelligence Screening Committee (2023-24)
- Member, Graduate Program Review Committee (Fall 2023)
- Panelist, NSF CAREER Writing Workshop (2023)
- Co-founder and Co-organizer, CWRU Chemistry Research Symposium (2023–)
- Panel Reviewer, Squire Scholarship Interview Panel (2023)
- Member, Graduate Admissions Committee (2019–)
- Co-chair, Colloquium Committee (2019–)
- Panel Reviewer, Expanding Horizons Initiative (2023)
- Member, Faculty Search Committee (AY2021-22)
- Member, Curriculum Committee (Fall 2020 (Sabbatical Replacement))
- Member, Chemistry Executive Committee (2019–2021)

professional service

peer review

- Physical Chemistry Chemical Physics (12)
- Journal of Physical Chemistry Letters (6)
- The Journal of Chemical Physics (5)
- Journal of Computational and Theoretical Chemistry (5)
- Nanoscale Advances (1)
- Inorganica Chimica Acta (1)
- The European Physical Journal B (1)
- Wiley Interdisciplinary Reviews (1)

grant review panels

- Department of Energy
- National Science Foundation

courses taught

- CHEM446/337: **Quantum Mechanics I** (3 credits) — Fall 2019, Fall 2021, Fall 2023
- CHEM447: **Modern Physical Chemistry (co-taught)** (3 credits) — Fall 2019, Fall 2022
- CHEM336: **Physical Chemistry II** (3 credits) — Spring 2020, Spring 2021, Spring 2023
- CHEM442/342: **Computational Chemistry** (3 credits) — Fall 2020, Fall 2022

advisees

postdoctoral researchers

- Dr. Anton Perera (2024 –)
- Dr. Sean Hoehn (2022 – 2024) — now at AkzoNobel
- Dr. Srijana Bhandari (2020 – 2022) — now at PNNL

Ph.D. students

- Abhijith Kumar (2021 –)
- Dehua Jiang (2022 –)
- Praseetha Prakash (2023 –)
- Mrigank Singh (2024 –)
- Qabas Alkhatib (2024 –)
- Ericka Miller (2019 – 2024) — now at Notre Dame
- John Zhou (2019 – 2023) — now at Changping National Laboratory

undergraduate students

- Thomas-Ethan Kaji (2022 –)
- William Kattner (2022 – 2023) — now at Medpace
- Annabella Debernardo (2019 – 2021) — now at UIUC
- Colin Schiltz (2019 – 2021) — now at UC Irvine
- Krista Schoonover (2020 – 2021) — now at Texas A&M

student awards

2023	Ericka Miller Best Presentation at 2023 Midwest Theoretical Chemistry Conference
2023	Ericka Miller Best Presentation at 2023 CWRU Chemistry Research Symposium
2023	Ericka Miller Molecular Sciences Software Institute (MolSSI) Software Fellowship