Shane M. Parker, PhD

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positions

2025 –	**Associate Professor** Case Western Reserve University	Cleveland, OH
2021 – 2025	**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 *Advisor*: Professor Filipp Furche	Irvine, CA
2009 – 2014	**PhD, Theoretical Chemistry** Northwestern University *Advisor*: Professor Mark Ratner and Professor Tamar Seideman	Evanston, IL
2008 – 2009	**Fulbright Fellow** Technische Universität München *Advisor*: Professor Notker Rösch	Munich, Germany
2004 – 2008	**B.S., Chemistry & B.S., Mathematics** University of Florida *Advisor*: 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

27 E. Roy Miller, S. M. Parker*,
Numerically Stable Resonating Hartree-Fock, *The Journal of Chemical Physics* **2025**, 104115, doi: 10.1063/5.0246790, 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 S_2 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.3c00

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

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

Before Case Western Reserve University

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 TiO_2 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	**PCCP Editor's choice**	Multi-state TDDFT paper selected as outstanding article by Editor-in-Chief

talks

Case Western Reserve University

February 3, 2025	**Simulating Photochemistry from First-Principles Quantum Chemistry *(invited)*** University of Houston	Houston, TX
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
August 29, 2024	**Simulating Photochemistry from First-Principles Quantum Chemistry *(invited)*** Case Western Reserve University	Cleveland, OH
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)*** Midwest Theoretical Chemistry Conference 2024	University of Wisconsin-Madison, Madison, WI
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, Massachussetts
August 2018	**Ensemble Optimized Time-Dependent Density Functional Theory *(invited)*** 256th American Chemical Society National Meeting and Exposition	Boston, Massachussetts
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, Spain
Benasque 9th TDDFT School

Before Case Western Reserve University

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

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:** FuSe2: Carbon Semiconductor Devices Based on γ-Graphyne
  Amount: $2,000,000 (17% Parker)
  Role: co-PI (PI: Valentin Rodionov)
  Source: NSF Future of Semiconductors (FuSe2)
  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