Shane M. Parker, PhD

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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 (Arnold O. Beckman Postdoctoral Fellow since 2016)** 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

publications

— W. B. Martin, S. M. Parker, V. Rodionov,
Errors in characterization and modeling undermine the report of the synthesis of γ-graphyne via alkyne metathesis, **2023**, under review

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

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

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

20 Z. Zhou, S. M. Parker,
Accelerating molecular property calculations with semiempirical preconditioning, *The Journal of Chemical Physics* **2021**, *155*, 204111

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

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

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

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

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

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

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

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

11 S. M. Parker, S. Roy, and F. Furche,
Unphysical divergences in response theory, *The Journal of Chemical Physics* **2016**, *145*, 134105

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

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

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

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

6 S. M. Parker, T. Shiozaki,
Quasi-diabatic states from active space decomposition, *Journal of Chemical Theory and Computation* **2014**, *10*, 3738

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

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

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

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

1 S. M. Parker, M. A. Ratner, T. Seideman,
Coherent control of molecular torsion, *The Journal of Chemical Physics* **2011**, *135*, 224301

book chapters

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

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**
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

current and pending support

- **Project Title:** Predictive tools for excited state chemistry
  Amount: $786,146
  Status: current
  Source: Case Western Reserve University
  Start Date: 07/2019
  Project Objective: Develop excited state electronic structure methods capable of powering nonadiabatic molecular dynamics simulations

- **Project Title:** Photochemistry with Resonating Mean-Field
  Amount: $650,000
  Status: current
  Source: NSF CAREER, Division of Chemistry (CHE)
  Start Date: 06/01/2023 **End Date:** 05/30/2028
  Project Objective: Develop algorithms and an implementation for the Resonating Mean-Field method towards establishing Resonating Mean-Field as a tool for photochemistry simulations
  Award ID: CHE-2236959

talks

September 2023	**Computational Photochemistry *(invited)*** Binghamton University, Department of Physics	Binghamton, NY
July 2023	**Fast spectra with the minimal auxiliary basis approach to TDDFT *(invited)*** Rutgers TDDFT Workshop	Rutgers, NJ
June 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
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

October 2022	**TDDFT in Chemistry and Biochemistry (2 lectures)** Benasque 9th TDDFT School	Benasque, Spain
July 2017	**Nonadiabatic molecular dynamics with TDDFT (2 lectures)** Telluride School on Time-dependent Density Functional Theory	Telluride, Colorado

courses taught

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

service

- Member, Chemistry Faculty Search Committee (AY2023-24)
- Member, CAS AI Search Committee (2023-24)
- Member, Graduate Program Review Committee (Fall 2023)
- Co-founder and Co-organizer, CWRU Chemistry Research Symposium (2023)
- Member, Chemistry Graduate Admissions Committee (2019–)
- Co-chair, Chemistry Colloquium Committee (2019–)
- Panel Reviewer, Expanding Horizons Initiative (2023)
- Member, Chemistry Faculty Search Committee (AY2021-22)
- Member, CAS Curriculum Committee (Fall 2020)

peer review

- Physical Chemistry Chemical Physics (10)
- Journal of Chemical Physics (4)
- Journal of Chemical Theory and Computation (3)
- Journal of Physical Chemistry Letters (3)
- Inorganica Chimica Acta (1)
- Nanoscale (1)
- Wiley Interdisciplinary Reviews-Computational Molecular Science (1)