Shane M. Parker, PhD

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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 (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

— 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
(2023), under review
Turbomole: Today and Tomorrow

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

22 Z. Zhou, F. Della Sala, S. M. Parker
The Journal of Physical Chemistry Letters, **14**, 1968-1976 (2023)
Minimal auxiliary basis set approach for the electronic excitation spectra of organic molecules

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
Journal of the American Chemical Society, **144**, 17999-18008 (2022)
Scalable Synthesis and Characterization of Multilayer γ-Graphyne, New Carbon Crystals with a Small Direct Band Gap

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

19 M. Gupta, M. Singha, D. Rasale, Z. Zhou, S. Bhandari, S. Beasley, J. Sakr, S. M. Parker, R. Spitale
Organic Letters, **23**, 7183-7187 (2021)
Mutually orthogonal bioconjugation of vinyl nucleosides for RNA metabolic labeling

18 J. Jimenez, Z. Zhou, A. L. Rheingold, S. M. Parker, G. Sauvé
Inorganic Chemistry, **60**, 13320-13331 (2021)

Tuning the properties of azadipyrromethene-based near-infrared dyes using intramolecular BO-chelation and peripheral substitutions

17 S. M. Parker, C. J. Schiltz
The Journal of Chemical Physics, **153**, 174109 (2020)
Surface hopping with cumulative probabilities: even sampling and improved reproducibility

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
The Journal of Chemical Physics, **152**, 184107 (2020)
TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations

15 S. M. Parker, S. Roy, F. Furche
Physical Chemistry Chemical Physics, **21**, 18999-19010 (2019)
Multistate hybrid time-dependent density functional theory with surface hopping accurately captures ultrafast thymine photodeactivation

14 M. Kubota, S. Nainar, S. M. Parker, W. England, F. Furche, R. Spitale
ACS Chemical Biology, **14**, 1698-1707 (2019)
Expanding the Scope of RNA Metabolic Labeling with Vinyl Nucleosides and Inverse Electron-Demand Diels-Alder Chemistry

13 S. M. Parker, D. Rappoport, F. Furche
Journal of Chemical Theory and Computation, **14**, 807-819 (2018)
Quadratic response properties from TDDFT: trials and tribulations

12 M. Muuronen, S. M. Parker, E. Berardo, A. Le, M. Zwijnenburg, F. Furche
Chemical Science, **8**, 2179-2183 (2017)
Mechanism of Photocatalytic Water Oxidation on Small TiO_2 Nanoparticles

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

10 V. A. Nasluzov, S. M. Parker, A. Genest, A. M. Shor, E. A. Ivanova-Shor, N. Rösch
Kinetics and Catalysis, **56**, 631 (2015)
Trinuclear tantalum clusters grafted to hydroxylated silica surfaces: A density-functional embedded-cluster study

9 I. Kim, S. M. Parker, T. Shiozaki
Journal of Chemical Theory and Computation, **11**, 3636 (2015)
Orbital Optimization in the Active Space Decomposition Model

8 S. M. Parker, T. Shiozaki
The Journal of Chemical Physics, **141**, 211102 (2014)
Active space Decomposition with multiple sites: Density matrix renormalization group algorithm

7 S. M. Parker, M. Smeu, I. Franco, M. A. Ratner, T. Seideman
Nano Letters, **14**, 4587 (2014)
Molecular Junctions: Can Pulling Influence Optical Controllability

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

5 S. M. Parker, T. Seideman, M. A. Ratner, T. Shiozaki
Journal of Physical Chemistry C, **118**, 12700 (2014)
Model Hamiltonian analysis of singlet fission from first principles

4 S. M. Parker, T. Seideman, M. A. Ratner, T. Shiozaki
The Journal of Chemical Physics, **139**, 021108 (2013)

Active-space decomposition for molecular dimers

3 Y. Wu, V. A. Karttunen, S. M. Parker, A. Genest, N. Rösch
Organometallics, **32**, 2363 (2013)
Olefin Hydrosilylation Catalyzed by a Bis-N-Heterocyclic Carbene Rhodium Complex. A Density Functional Theory Study

2 S. M. Parker, M. A. Ratner, T. Seideman
Molecular Physics, **110**, 1941 (2012)
Simulating strong field control of axial chirality using optimal control theory

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

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

- **Project Title:** Fast nonlinear properties calculations for predicted transient spectra through a minimal-auxiliary basis set method
  Amount: $100,000
  Status: declined
  Source: Camille Dreyfus Teacher-Scholar Awards Program
  Project Objective: We will develop a fast approximation for predicting nonlinear and transient spectra from first-principles time-dependent density functional theory (TDDFT), called TDDFT-ris, that will retain the high accuracy of TDDFT but reduce the computational cost by several orders of magnitude.

invited lectures

July 2023	**Fast spectra with the minimal auxiliary basis approach to TDDFT** Rutgers TDDFT Workshop	Rutgers, NJ
October 2022	**Fast Spectra with the minimal auxiliary basis approach to TDDFT** Benasque 9th TDDFT Workshop	Benasque, Spain
August 2022	**Accelerating Quantum Chemistry with Semiempirical Preconditioning** CWRU-Tohoku 8th Annual Data Science in Engineering and Life Sciences Symposium	Cleveland, Ohio
August 2018	**Excited-State Chemistry with TDDFT** 256th American Chemical Society National Meeting and Exposition	Boston, Massachussetts
August 2018	**Ensemble Optimized Time-Dependent Density Functional Theory** 256th American Chemical Society National Meeting and Exposition	Boston, Massachussetts
July 2017	**Nonlinear properties from TDDFT: trials and tribulations** Excited States: Electronic Structure and Dynamics	Telluride, Colorado
April 2017	**Nonlinear properties from TDDFT: trials and tribulations** 253rd American Chemical Society National Meeting and Exposition	San Francisco, California
June 2015	**Non-adiabatic molecular dynamics** 98th Meeting of the Canadian Society of Chemistry	Ottawa, Ontario
June 2014	**Model Hamiltonians from the Active-space Decomposition Method** 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)