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## positions

|             |                                                                                                                                                            |                 |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
| 2021 –      | <b>Frank Hovorka Assistant Professor of Chemistry</b><br>Case Western Reserve University                                                                   | Cleveland, OH   |
| 2019 – 2021 | <b>Assistant Professor of Chemistry</b><br>Case Western Reserve University                                                                                 | Cleveland, OH   |
| 2014 – 2019 | <b>Postdoctoral Fellow (Arnold O. Beckman Postdoctoral Fellow since 2016)</b><br>University of California Irvine<br><i>Advisor:</i> Professor Filip Furche | Irvine, CA      |
| 2009 – 2014 | <b>PhD, Theoretical Chemistry</b><br>Northwestern University<br><i>Advisor:</i> Professor Mark Ratner and Professor Tamar Seideman                         | Evanston, IL    |
| 2008 – 2009 | <b>Fulbright Fellow</b><br>Technische Universität München<br><i>Advisor:</i> Professor Notker Rösch                                                        | Munich, Germany |
| 2004 – 2008 | <b>B.S., Chemistry &amp; B.S., Mathematics</b><br>University of Florida<br><i>Advisor:</i> 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  $\gamma$ -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  $\gamma$ -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 azadipyromethene-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<sub>2</sub> 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 | <b>Scilight featured article</b> | Photochemistry simulations dramatically improve reliability and reproducibility |
| 2020 | <b>JCP Editor's choice</b>       | Cumulative surface hopping paper highlighted by AIP                             |
| 2019 | <b>PCCP Editor's choice</b>      | Multi-state TDDFT paper selected as outstanding article by Editor-in-Chief      |

## awards

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

## invited lectures

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

## pedagogical lectures

|              |                                                                                                                                |                     |
|--------------|--------------------------------------------------------------------------------------------------------------------------------|---------------------|
| October 2022 | <b>TDDFT in Chemistry and Biochemistry (2 lectures)</b><br>Benasque 9th TDDFT School                                           | Benasque, Spain     |
| July 2017    | <b>Nonadiabatic molecular dynamics with TDDFT (2 lectures)</b><br>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)