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

— V. G. Desyatkin, W. B. Martin, E. Roy Miller, F. Ted Limpoco, S. R. Almahdali, S. M. Parker, V. O. Rodionov (2022), submitted
Synthesis and Characterization of Multilayer Graphyne, a Novel Allotrope of Carbon

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 – 2024	**Frank Hovorka Professor of Chemistry, CWRU**
2020 – 2021	**Glennan Fellowship, CWRU**
2020	**STAIR Mentor Fellows Program, CWRU**
2019	**Nominated for 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	**Lindau Conference** selected to attend conference bringing together young researchers and Nobel laureates
2008 – 2009	**Fulbright Fellowship** Technische Universität München
2006	**Anderson Scholar with Highest Distinction** for academic achievement and uninterrupted study

invited lectures

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

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)
- CHEM447: **Modern Physical Chemistry (co-taught)** (Fall 2019)
- CHEM336: **Physical Chemistry II** (Spring 2020, 2021)
- CHEM442/342: **Computational Chemistry** (Fall 2020)