

Shane M. Parker

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positions

2019 –	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 <i>Advisor:</i> Professor Filipp Furche	Irvine, CA
2009 – 2014	PhD, Theoretical Chemistry Northwestern University <i>Advisor:</i> Professor Mark Ratner and Professor Tamar Seideman	Evanston, IL
2008 – 2009	Fulbright Fellow Technische Universität München <i>Advisor:</i> Professor Notker Rösch	Munich, Germany
2004 – 2008	B.S., Chemistry & B.S., Mathematics University of Florida <i>Advisor:</i> Professor N. Yngve Öhrn	Gainesville, FL

publications

- 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. Zwiijnenburg, F. Furche
Chemical Science, **8**, 2179-2183 (2017)
Mechanism of Photocatalytic Water Oxidation on Small TiO₂ 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
2019	PCCP Editor's choice	Multi-state TDDFT paper selected as outstanding article by Editor-in-Chief

awards

2020	Glennan Fellowship
2016 – 2019	Arnold O. Beckman Postdoctoral Fellowship
2010 – 2013	Department of Energy Office of Science Graduate Fellowship
2008 – 2009	Fulbright Fellowship Technische Universität München

invited lectures

August 2018	Excited-State Chemistry with TDDFT 256th American Chemical Society National Meeting and Exposition	Boston, Massachusetts
August 2018	Ensemble Optimized Time-Dependent Density Functional Theory 256th American Chemical Society National Meeting and Exposition	Boston, Massachusetts
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
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select teaching

Fall 2020	Computational Chemistry (CHEM342/442)	Undergraduate + Graduate, CWRU
Spring 2020	Physical Chemistry II (CHEM336)	Undergraduate, CWRU
Fall 2019	Introduction to Quantum Mechanics (CHEM446)	Undergraduate + Graduate, CWRU
2015	Computational Chemistry	Undergraduate + Graduate, UC Irvine
2013	Quantum Chemistry	Graduate course, Northwestern University
2011	Introduction to Quantum Chemistry	Undergraduate course, Northwestern University
2009	Computational Chemistry	Undergraduate course, Technische Universität München
2008	Introduction to Quantum Mechanics	Undergraduate course, Technische Universität München