Shane M. Parker

e-mail: shane.parker@case.edu
web: quantumparker.com
ph: (216) 368-3697

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 *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

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

2019 **PCCP Editor's choice** Multi-state TDDFT paper selected as outstanding article by Editor-in-Chief

awards

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, 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

select teaching

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