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 *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

— S. M. Parker, S. Roy, F. Furche
Physical Chemistry Chemical Physics, (2019), accepted
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

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

Fall 2019	Instructor for **Quantum Mechanics** Undergraduate + Graduate, CWRU
2015	Guest Lecturer (2 lectures) for **Computational Chemistry** Undergraduate + Graduate, UC Irvine
2013	Teaching Assistant for **Quantum Chemistry** Graduate course, Northwestern University
2011	Teaching Assistant for **Introduction to Quantum Chemistry** Undergraduate course, Northwestern University
2009	Teaching Assistant for **Computational Chemistry** Undergraduate course, Technische Universität München
2008	Teaching Assistant for **Introduction to Quantum Mechanics** Undergraduate course, Technische Universität München