EDWARD G. HOHENSTEIN

PULSE Institute for Ultrafast Energy Sciences, Energy Sciences Directorate
SLAC National Accelerator Laboratory
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Menlo Park, CAS 94025

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CURRENT POSITION

Senior Staff Scientist, 2018 to present
PULSE Institute for Ultrafast Energy Sciences
SLAC National Accelerator Laboratory, Menlo Park, CA

PREVIOUS POSITIONS

Assistant Professor, 2014 to 2019
Department of Chemistry and Biochemistry
City College of New York, New York, NY

EDUCATION

Washington College, Chestertown, MD
Bachelor of Science, *summa cum laude*, May 2007
Majors in Chemistry and Mathematics

Georgia Institute of Technology, Atlanta, GA
Doctor of Philosophy, December 2011
Graduate Advisor: Prof. C. David Sherrill

Postdoctoral Researcher, 2011 to 2014
Stanford University, Stanford, CA
Postdoctoral Advisor: Prof. Todd J. Martínez

PUBLICATIONS

60. "Rank reduced coupled cluster theory. II. Equation-of-motion coupled-cluster singles and doubles," E. G. Hohenstein, Y. Zhao, R. M. Parrish, and T. J. Martínez, *J. Chem. Phys.*, **151**, 164121 (2019)
59. "Quantum Computation of Electronic Transitions using a Variational Quantum Eigensolver," R. M. Parrish, E. G. Hohenstein, P. L. McMahon and T. J. Martínez, *Phys. Rev. Lett.*, **122**, 230401 (2019)
58. "Rank reduced coupled cluster theory. I. Ground state energies and wavefunctions," R. M. Parrish, Y. Zhao, E. G. Hohenstein, and T. J. Martínez, *J. Chem. Phys.*, **150**, 164118 (2019)
57. "Nature-Derived Sodium-Ion Battery: Mechanistic Insights into Na-Ion Coordination within Sustainable Molecular Cathode Materials," M. Miroshnikov, K. Kato, G. Babu, N. K. Thangavel, K. Mahankali, E. G. Hohenstein, H. Wang, S. Satapathy, K. P. Divya, H. Asare, L. M. R. Arava, P. M. Ajayan, and G. John *ACS Appl. Energy Mater.*, **2**, 8596 (2019)
56. "Made From Henna! A Fast-Charging, High-Capacity, and Recyclable Tetrakislawsone Cathode Material for Lithium Ion Batteries," M. Miroshnikov, K. Kato, G. Babu, N. K. Thangavel, K. Mahankali, E. G. Hohenstein, H. Wang, S. Satapathy, K. P. Divya, H. Asare, P. M. Ajayan, L. M. R. Arava, and G. John *ACS Sustainable Chem. Eng.*, **7**, 13836 (2019)

55. "Stereoisomer Specific Reaction of Hexabromocyclododecane with Reduced Sulfur Species in Aqueous Solutions," X. Zhang, J. H. Wilson, A. J. Lawson, E. G. Hohenstein, and U. Jans, *Chemosphere*, **226**, 238 (2019)

54. "Effect of Non-Planarity on Excited-State Proton Transfer and Internal Conversion in Salicylideneaniline," S. Pijeau, D. Foster, and E. G. Hohenstein, *J. Phys. Chem. A* **122**, 5555 (2018)

53. "Nonadiabatic Ab Initio Molecular Dynamics with the Floating Occupation Molecular Orbital-Complete Active Space Configuration Interaction Method," *J. Chem. Theory Comput.* D. Hollas, L. Šištík, E. G. Hohenstein, T. J. Martínez, and P. Slavíček, **14**, 339 (2018)

52. "Complete Active Space Configuration Interaction from State-Averaged Configuration Interaction Singles Natural Orbitals: Analytic First Derivatives and Derivative Coupling Vectors," B. S. Fales, Y. Shu, B. G. Levine, and E. G. Hohenstein, *J. Chem. Phys.* **147**, 094104 (2017)

51. "Excited-State Dynamics of a Benzotriazole Photostabilizer: 2-(2′-Hydroxy-5′-methylphenyl)benzotriazole," S. Pijeau, D. Foster, and E. G. Hohenstein, *J. Phys. Chem. A* **121**, 6377 (2017)

50. "Robust and Efficient Spin Purification for Determinantal Configuration Interaction," B. S. Fales, E. G. Hohenstein, and B. G. Levine, *J. Chem. Theory Comput.* **13**, 4162 (2017)

49. "Excited-State Dynamics of 2-(2′-Hydroxyphenyl)Benzothiazole: Ultrafast Proton Transfer and Internal Conversion," S. Pijeau, D. Foster, and E. G. Hohenstein, *J. Phys. Chem. A* **121**, 4595 (2017)

48. "Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability," R. M. Parrish *et al.*, *J. Chem. Theory Comput.* **13**, 3185 (2017)

47. "Atomistic Non-Adiabatic Dynamics of the LH2 Complex with a GPU-Accelerated *Ab Initio* Exciton Model," A. Sisto, C. Stross, M. W. van der Kamp, M. O'Connor, S. McIntosh-Smith, G. T. Johnson, E. G. Hohenstein, F. R. Manby, D. R. Glowacki, and T. J. Martínez, *Phys. Chem. Chem. Phys.* **19**, 14924 (2017)

46. "A Direct-Compatible Formulation of the Coupled Perturbed Complete Active Space Self-Consistent Field Equations on Graphical Processing Units," J. W. Snyder, B. S. Fales, E. G. Hohenstein, B. G. Levine, and T. J. Martínez, *J. Chem. Phys.* **146**, 174113 (2017)

45. "Improved Complete Active Space Configuration Interaction Energies with a Simple Correction from Density Functional Theory," S. Pijeau and E. G. Hohenstein, *J. Chem. Theory Comput.* **13**, 1130 (2017)

44. "Analytic Formulation of Derivative Coupling Vectors for Complete Active Space Configuration Interaction Wavefunctions with Floating Occupation Molecular Orbitals," E. G. Hohenstein, *J. Chem. Phys.* **145**, 174110 (2016)

43. " "Balancing" the Block Davidson–Liu Algorithm," R. M. Parrish, E. G. Hohenstein, and T. J. Martínez, *J. Chem. Theory Comput.* **12**, 3003 (2016)

42. "Mechanism for the Enhanced Excited-State Lewis Acidity of Methyl Viologen," E. G. Hohenstein, *J. Am. Chem. Soc.* **138**, 1868 (2016)

41. "Competition Between π-π and C-H/π Interactions: A Comparison of the Structural and Electronic Properties of Alkoxy-Substituted 1,8-bis((Propyloxyphenyl)ethynyl)naphthalenes," B. E. Carson, T. M. Parker, E. G. Hohenstein, G. L. Brizius, W. Komorner, R. A. King, D. M. Collard, and C. D. Sherrill, *Chem. Eur. J.* **21**, 19168 (2015)

40. "An Atomic Orbital-Based Formulation of Analytical Gradients and Nonadiabatic Coupling Vector Elements for the State-Averaged Complete Active Space Self-Consistent Field Method on Graphical Processing Units," J. W. Snyder, E. G. Hohenstein, N. Luehr, and T. J. Martínez, *J. Chem. Phys.* **143**, 154107 (2015)

39. "Analytic First Derivatives of Floating Occupation Molecular Orbital-Complete Active Space Configuration Interaction on Graphical Processing Units," E. G. Hohenstein, M. E. F. Bouduban, C. Song, N. Luehr, I. S. Ufimtsev, and T. J. Martínez, *J. Chem. Phys.* **143**, 014111 (2015)

38. "An Atomic Orbital-Based Formulation of the Complete Active Space Self-Consistent Field Method on Graphical Processing Units," E. G. Hohenstein, N. Luehr, I. S. Ufimtsev, and T. J. Martínez, *J. Chem. Phys.* **142**, 224103 (2015)

37. "Tensor Hypercontraction Second-Order Møller-Plesset Perturbation Theory: Grid Optimization and Reaction Energies," S. I. L. Kokkila Schumacher, E. G. Hohenstein, R. M. Parrish, L.-P. Wang, and T. J. Martínez, *J. Chem. Theory Comput.* **11**, 3042 (2015)

36. "Determination of Hydrogen Bond Structure in Water Versus Aprotic Environments to Test the Relationship Between Length and Stability," P. A. Sigala, E. A. Ruben, C. W. Liu, P. M. B. Piccoli, E. G. Hohenstein, T. J. Martínez, A. J. Schultz, and D. Herschlag, *J. Am. Chem. Soc.* **137**, 5730 (2015)

35. "Configuration Interaction Singles Natural Orbitals: An Orbital Basis for an Efficient and Size Intensive Multireference Description of Electronic Excited States," Y. Shu, E. G. Hohenstein, and B. G. Levine, *J. Chem. Phys.* **142**, 024102 (2015)

34. "Advances in Molecular Quantum Chemistry Contained in the Q-Chem 4 Program Package," Y. Shao *et al.*, *Mol. Phys.* **113**, 184 (2015)

33. "Rotational State Analysis of AlH^+ by Two-Photon Dissociation," C. M. Seck, E. G. Hohenstein, C.-Y. Lien, P. R. Stollenwerk, and B. C. Odom, *J. Mol. Spectrosc.* **300**, 108 (2014)

32. "Communication: Acceleration of Coupled Cluster Singles and Doubles via Orbital-Weighted Least-Squares Tensor Hypercontraction," R. M. Parrish, C. D. Sherrill, E. G. Hohenstein, S. I. L. Kokkila, and T. J. Martínez, *J. Chem. Phys.* **140**, 181102 (2014)

31. "Tractability Gains in Symmetry-Adapted Perturbation Theory Including Coupled Double Excitations: CCD+ST(CCD) Dispersion with Natural Orbital Truncations," R. M. Parrish, E. G. Hohenstein, and C. D. Sherrill, *J. Chem. Phys.* **139**, 174102 (2013)

30. "Exact Tensor Hypercontraction: A Universal Technique for the Resolution of Matrix Elements of Local Finite-Range N-Body Potentials in Many-Body Quantum Problems," R. M. Parrish, E. G. Hohenstein, N. F. Schunck, C. D. Sherrill, and T. J. Martínez, *Phys. Rev. Lett.* **111**, 132505 (2013)

29. "Tensor Hypercontraction Equation-of-Motion Second-Order Approximate Coupled Cluster: Electronic Excitation Energies in $\mathcal{O}(N^4)$ Time," E. G. Hohenstein, S. I. L. Kokkila, R. M. Parrish, and T. J. Martínez, *J. Phys. Chem. B* **117**, 12972 (2013)

28. "Discrete Variable Representation in Electronic Structure Theory: Quadrature Grids for Least-Squares Tensor Hypercontraction," R. M. Parrish, E. G. Hohenstein, T. J. Martínez, and C. D. Sherrill, *J. Chem. Phys.* **138**, 194107 (2013)

27. "Quartic Scaling Second-Order Approximate Coupled Cluster Singles and Doubles via Tensor Hypercontraction: THC-CC2," E. G. Hohenstein, S. I. L. Kokkila, R. M. Parrish, and T. J. Martínez, *J. Chem. Phys.* **138**, 124111 (2013)

26. "Quantum-Mechanical Analysis of the Energetic Contributions to π Stacking in Nucleic Acids versus Rise, Twist, and Slide," T. M. Parker, E. G. Hohenstein, R. M. Parrish, N. V. Hud, and C. D. Sherrill, *J. Am. Chem. Soc.* **135**, 1306 (2013)

25. "Communication: Tensor Hypercontraction. III. Least-Squares Tensor Hypercontraction for the Determination of Correlated Wavefunctions," E. G. Hohenstein, R. M. Parrish, C. D. Sherrill, and T. J. Martínez, *J. Chem. Phys.* **137**, 221101 (2012)

24. "Tensor Hypercontraction. II. Least-Squares Renormalization," R. M. Parrish, E. G. Hohenstein, T. J. Martínez, and C. D. Sherrill, *J. Chem. Phys.* **137**, 224106 (2012)

23. "Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set," J. C. Flick, D. Kosenkov, E. G. Hohenstein, C. D. Sherrill, and L.V. Slipchenko, *J. Chem. Theory Comput.* **8**, 2835 (2012)

22. "Tensor Hypercontraction Density Fitting. I. Quartic Scaling Second- and Third-Order Møller-Plesset Perturbation Theory," E. G. Hohenstein, R. M. Parrish, and T. J. Martínez, *J. Chem. Phys.* **137**, 044103 (2012)

21. "PSI4: An Open-Source *Ab Initio* Electronic Structure Program," J. M. Turney, A. C. Simmonett, R. M. Parrish, E. G. Hohenstein, F. Evangelista, J. T. Fermann, B. J. Mintz, L. A. Burns, J. J. Wilke, M. L. Abrams, N. J. Russ, M. L. Leininger, C. L. Janssen, E. T. Seidl, W. D. Allen, H. F. Schaefer, R. A. King, E. F. Valeev, C. D. Sherrill, and T. D. Crawford, *WIREs Comput. Mol. Sci.* **2**, 556 (2012)

20. "Wavefunction Methods for Noncovalent Interactions," E. G. Hohenstein and C. D. Sherrill, *WIREs Comput. Mol. Sci.* **2**, 304 (2012)

19. "Role of Long-Range Intermolecular Forces in the Formation of Inorganic Nanoparticle Clusters," G. V. Gibbs, T. D. Crawford, A. F. Wallace, D. F. Cox, R. M. Parrish, E. G. Hohenstein, and C. D. Sherrill, *J. Phys. Chem. A* **115**, 12933 (2011)

18. "Large-Scale Symmetry-Adapted Perturbation Theory Computations Via Density Fitting and Laplace Transformation Techniques: Investigating the Fundamental Forces of DNA-Intercalator Interactions," E. G. Hohenstein, R. M. Parrish, C. D. Sherrill, J. M. Turney, and H. F. Schaefer, *J. Chem. Phys.* **135**, 174107 (2011)

17. "Structures of Protonated Benzene Dimer and Intermolecular Interaction Decomposition Via Symmetry-Adapted Perturbation Theory," H. M. Jaeger, H. F. Schaefer, E. G. Hohenstein, and C. D. Sherrill, *Comput. Theor. Chem.* **973**, 47 (2011)

16. "Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P_2, and PCCP," E. G. Hohenstein, H. M. Jaeger, E. J. Carrell, G. S. Tschumper, and C. D. Sherrill, *J. Chem. Theory Comput.* **7**, 2842 (2011)

15. "Origin of the Surprising Enhancement of Electrostatic Energies by Electron-Donating Substituents in Substituted Sandwich Benzene Dimers," E. G. Hohenstein, J. Duan, and C. D. Sherrill, *J. Am. Chem. Soc.* **133**, 13244 (2011)

14. "Challenges of Laser-cooling Molecular Ions," J. H. V. Nguyen, C. R. Viteri, E. G. Hohenstein, C. D. Sherrill, K. R. Brown, and B. Odom, *New. J. Phys.* **13**, 063023 (2011)

13. "Assessment of the Performance of DFT and DFT-D Methods for Describing Distance Dependence of Hydrogen-Bonded Interactions," K. S. Thanthiriwatte, E. G. Hohenstein, L. A. Burns, and C. D. Sherrill, *J. Chem. Theory Comput.* **7**, 88 (2011)

12. "Efficient Evaluation of Triple Excitations in Symmetry-Adapted Perturbation Theory Via Second-Order Møller-Plesset Perturbation Theory Natural Orbitals," E. G. Hohenstein and C. D. Sherrill, *J. Chem. Phys.* **133**, 104107 (2010)

11. "Density Fitting of Intramonomer Correlation Effects in Symmetry-Adapted Perturbation Theory," E. G. Hohenstein and C. D. Sherrill, *J. Chem. Phys.* **133**, 014101 (2010)

10. "Density Fitting and Cholesky Decomposition Approximations in Symmetry-Adapted Perturbation Theory: Implementation and Application to Probe the Nature of π-π Interactions in Linear Acenes," E. G. Hohenstein and C. D. Sherrill, *J. Chem. Phys.* **132**, 184111 (2010)

9. "Basis Set Consistent Revision of the S22 Test Set of Noncovalent Interaction Energies," T. Takatani, E. G. Hohenstein, M. Malagoli, M. S. Marshall, and C. D. Sherrill, *J. Chem. Phys.* **132**, 144104 (2010)

8. "Accurately Characterizing the π-π Interaction Energies of Indole-Benzene Complexes," Y. Geng, T. Takatani, E. G. Hohenstein, and C. D. Sherrill, *J. Phys. Chem. A* **114**, 3576 (2010)

7. "Assessment of Standard Force Field Models Against High-Quality Ab Initio Potential Curves for Prototypes of π-π, CH/π, and SH/π Interactions," C. D. Sherrill, B. G. Sumpter, M. O. Sinnokrot, M. S. Marshall, E. G. Hohenstein, R. C. Walker, and I. R. Gould, *J. Comput. Chem.* **30**, 2187 (2009)

6. "An Assessment of Theoretical Methods for Nonbonded Interactions: Comparison to Complete Basis Set Limit Coupled-Cluster Potential Energy Curves for the Benzene Dimer, the Methane Dimer, Benzene-Methane, and Benzene-H_2S," C. D. Sherrill, T. Takatani, and E. G. Hohenstein, *J. Phys. Chem. A* **113**, 10146 (2009)

5. "Reactive Desorption Electrospray Ionization Mass Spectrometry (DESI-MS) of Natural Products of Marine Alga," L. Nyadong, E. G. Hohenstein, A. Galhena, A. L. Lane, J. Kubanek, C. D. Sherrill, and F. M. Fernandez, *Anal. Bioanal. Chem.* **394**, 245 (2009)

4. "Effects of Heteroatoms On Aromatic π-π Interactions: Benzene-Pyridine and Pyridine Dimer," E. G. Hohenstein and C. D. Sherrill, *J. Phys. Chem. A* **113**, 878 (2009)
3. "Assessment of the Performance of the M05-2X and M06-2X Exchange-Correlation Functionals for Noncovalent Interactions in Biomolecules," E. G. Hohenstein, S. T. Chill, and C. D. Sherrill, *J. Chem. Theory Comput.* **4**, 1996 (2008)
2. "Desorption Electrospray Ionization Reactions Between Host Crown Ethers and the Influenza Neuraminidase Inhibitor Oseltamivir for the Rapid Screening of Tamiflu," L. Nyadong, E. G. Hohenstein, K. Johnson, C. D. Sherrill, M. D. Green, and F. M. Fernandez, *Analyst* **133**, 1513 (2008)
1. "Improvement of the Coupled-Cluster Singles and Doubles Method Via Scaling Same- and Opposite-Spin Components of the Double Excitation Correlation Energy," T. Takatani, E. G. Hohenstein, and C. D. Sherrill, *J. Chem. Phys.* **128**, 124111 (2008)

TEACHING EXPERIENCE

Fall 2014, Chem 10401, General Chemistry II

Fall 2015, Chem 33200, Physical Chemistry II

Fall 2016, Chem 33200, Physical Chemistry II

Fall 2016, Chem 43400, Physical Chemistry and Chemical Instrumentation Laboratory II

Spring 2017, Chem 33200, Physical Chemistry II

Spring 2017, Chem 43400, Physical Chemistry Laboratory I

Fall 2017, Chem 33200, Physical Chemistry II

Fall 2017, Chem 43400, Physical Chemistry and Chemical Instrumentation Laboratory II

Spring 2018, Chem 33200, Physical Chemistry II

Spring 2018, Chem 43400, Physical Chemistry Laboratory I

INVITED TALKS

"Hybrid Quantum/Classical Computation for Large-Scale Chemical Simulation," E. G. Hohenstein, Q2B 2019: Practical Quantum Computing, San Jose, CA (2019)

"First Principles Simulation of Excited-State Proton Transfer," E. G. Hohenstein, 29th International Conference on Photochemistry, Boulder, CO (2019)

"A Unified Low-Rank Formulation of Coupled-Cluster Theory," E. G. Hohenstein, Computational and Theoretical Chemistry PI Meeting, Gaithersburg, MD (2019)

"Nonadiabatic Dynamics of Excited-State Proton Transfer," E. G. Hohenstein, Department of Chemistry, Binghamton University, Binghamton, New York, (2019)

"Efficient simulation of nonadiabatic dynamics via density functional embedding," E. G. Hohenstein, CI:NYU Conical Intersections, New York University, New York, New York, (2017)

"Nonadiabatic dynamics of excited-state proton transfer," E. G. Hohenstein, Department of Chemistry, William Patterson University, Montclair, NJ, (2017)

"Nonadiabatic dynamics using multiconfigurational wavefunctions with embedding corrections from density functional theory," E. G. Hohenstein, Fall National Meeting of the American Chemical Society, (2017)

"Photochemical dynamics via multiconfigurational wavefunction-in-DFT embedding," E. G. Hohenstein, New York Theoretical and Computational Chemistry Conference, (2016)

"First principles simulation of excited state proton transfer," E. G. Hohenstein, Department of Chemistry and Biochemistry, Queens College, New York, New York, (2016)

"Nonadiabatic Dynamics with Complete Active Space Methods and Graphical Processing Units," E. G. Hohenstein, ACS Northeast Regional Meeting, (2016)

"Nonadiabatic Dynamics from First Principles on Graphical Processing Units," E. G. Hohenstein, 8th Molecular Quantum Mechanics, Uppsala, Sweden, (2016)

"The Surprising Photochemistry of Aqueous Methyl Viologen," E. G. Hohenstein, Department of Chemistry and Biochemistry, The City College of New York, New York, New York, (2016)

"Multiconfigurational Quantum Chemistry on GPUs: Simulating Photoacids in the Condensed Phase," E. G. Hohenstein, Excited States and Time-Dependent Electronic Structure Theory, Telluride Science Research Center, (2015)

"Multiconfigurational Quantum Chemistry on Graphical Processing Units," E. G. Hohenstein, Department of Physics, The City College of New York, New York, New York, (2015)

"Computational Photochemistry in the Condensed Phase using Graphical Processing Units," E. G. Hohenstein, Department of Chemistry, College of Staten Island, New York, New York, (2015)

"Accelerating Multiconfigurational Quantum Chemistry with Graphical Processing Units," E. G. Hohenstein, International Workshop on Massively Parallel Programming, Tokyo, Japan, (2014)

"Approximations to the Complete Active Space Self-Consistent Field Method for Excited State Molecular Dynamics," E. G. Hohenstein, Association of Theoretical and Computational Chemistry at CUNY, Fall Workshop, (2014)

"Reduced Scaling in Electronic Structure Theory via Tensor Hypercontraction," E. G. Hohenstein, R. M. Parrish, and T. J. Martínez, Fall National Meeting of the American Chemical Society, (2014)

"Tensor Hypercontraction and Graphical Processing Units for Electronic Structure Theory," E. G. Hohenstein, S. I. L. Kokkila, R. M. Parrish, and T. J. Martínez, SIAM Conference on Parallel Processing for Scientific Computing, (2014)

"Reduced Scaling in Coupled-Cluster Theory via Tensor Hypercontraction," E. G. Hohenstein, S. I. L. Kokkila, R. M. Parrish, C. D. Sherrill, and T. J. Martínez, High-Performance Tensor Software for Scientific Computing, (2013)

"Reduced Scaling in Electronic Structure Theory via Tensor Hypercontraction," E. G. Hohenstein, R. M. Parrish, and T. J. Martínez, 12th U.S. National Congress on Computational Mechanics, (2013)

"The Origins of Noncovalent Forces in Biological Macromolecules," E. G. Hohenstein and C. D. Sherrill, Chemistry and Biochemistry Graduate Research Symposium, Georgia Tech, (2010)

CONTRIBUTED TALKS

"The Photo-Enhanced Lewis Acidity of Aqueous Methyl Viologen," E. G. Hohenstein, ACS Middle Atlantic Regional Meeting, (2016)

"Multiconfigurational Quantum Chemistry on Graphical Processing Units," E. G. Hohenstein, ACS Middle Atlantic Regional Meeting, (2016)

"Multiconfigurational Quantum Chemistry on Graphical Processing Units," E. G. Hohenstein, Fall National Meeting of the American Chemical Society, (2015)

"Density Fitting and Cholesky Decomposition Approximations in Symmetry-Adapted Perturbation Theory," E. G. Hohenstein and C. D. Sherrill, Meeting of the Southeastern Theoretical Chemistry Association, (2010)

CURRENT FUNDING

(co-PI) 9/1/19 - 8/31/22
DOE (FWP #100541)
"Hybrid Quantum/Classical Algorithms for Photochemistry and Nonadiabatic Dynamics"

(co-PI) 9/30/17 - 9/30/21
DOE (FWP #100384)
"SciDAC: Designing Photocatalysts Through Scalable Quantum Mechanics and Dynamics"

PAST FUNDING

68875-00 46 (PI) 7/1/15 - 12/31/16
PSC-CUNY $12,000
"Probing Photoacidity in Cyanonaphthols with ab initio Molecular Dynamics"

69805-00 47 (PI) 7/1/16 - 12/31/17
PSC-CUNY $5,998.58
"Nonadiabatic Dynamics via Complete Active Space Configuration Interaction Methods Accelerated with Graphical Processing Units"

D01_W911SR-14-2-0001-0008 (co-PI) 3/8/16 - 3/8/17
US Army, Defense Threat Reduction Agency
Minority Serving Institutions Science, Technology, Engineering and Mathematics Research and Development Consortium (MSRDC) $101,764
"Using the Hard and Soft, Acids and Bases (HSAB) Theory to Predict Organophosphate Target Interactions"

60719-00 48 (PI) 7/1/17 - 6/30/18
PSC-CUNY $5,998.58
"Excited-state dynamics of hydroxyphenyl-benzotriazole photostabilizers"

D01_W911SR-14-2-0001-0020 (co-PI) 8/17/17 - 8/16/18
US Army, Defense Threat Reduction Agency
Minority Serving Institutions Science, Technology, Engineering and Mathematics Research and Development Consortium (MSRDC) $120,815
"Using the Hard and Soft, Acids and Bases (HSAB) Theory to Predict Organophosphate Target Interactions"