Curriculum Vitae
Joseph Eli Subotnik
July, 2016.

1. Joseph E. Subotnik: Professor, Chemistry Department
email: subotnik@sas.upenn.edu

2. Work Address:
University of Pennsylvania
Department of Chemistry
231 S. 34th Street
Philadelphia, PA 19104

3. Education:
B.A. Harvard University *summa cum laude*, June, 2000. Physics and Math.
Ph.D. (Biophysics) UC Berkeley. September, 2001- December, 2006.
Ph.D. Advisor: Martin Head-Gordon.

4. Research and Professional Experience
- July 2016 – present, Professor, Chemistry Department, University of Pennsylvania.
- July 2014 – June 2016, Associate Professor, Chemistry Department, University of Pennsylvania.
- July 2010 – June 2014, Assistant Professor, Chemistry Department, University of Pennsylvania.
- July 2009 – June 2010, Postdoctoral Research Fellow Northwestern University.
  Advisor: Mark Ratner.
- July 2007 – June 2009, NSF International Postdoctoral Fellow. Tel-Aviv University.
  Advisor: Abraham Nitzan.
- January 2007 - June 2007, Postdoctoral Researcher, UC Berkeley.
  Advisor: Martin Head-Gordon.

5. Awards and Honors
2016: Guggenheim Fellowship
2015: Camille and Henry Dreyfus Teacher Scholar Award
2015: Journal of Physical Chemistry *B* Lectureship
2013: Research Corporation Cottrell Scholar
2012: Packard Fellowship for Science and Engineering
2012: Presidential Early Career Award for Science and Engineering (PECASE)
2012: NSF CAREER Award
2012: Alfred P. Sloan Research Fellow
2012: ACS Hewlett-Packard Outstanding Junior Faculty Award
2011: Air Force Young Investigator
2009: ACS Postdoctoral Highlighted Fellow in Physical Chemistry
2007-2009: NSF International Postdoctoral Fellow, Tel-Aviv University
2001-2006: John and Fannie Hertz Foundation Fellowship in Applied Sciences.
Fellowship at Berkeley University.

2000: B.A. Harvard University, *Summa Cum Laude.*
1999: Junior *Phi Beta Kappa*, Harvard University.

6. Funding:
Camille and Henry Dreyfus Teacher Scholar Award (2015-2017)

Research Corporation Cottrell Scholar Fellowship (2014-2017)

Packard Fellowship for Science and Engineering: (2012-2017)

Alfred P. Sloan Research Fellowship (2012-2014)

National Science Foundation (2012-2017)

- NSF CAREER: "Quantum Chemistry for Predicting and Quantifying Photoinduced Nonadiabatic Dynamics" (2012-2017)

Air Force Office of Scientific Research:(2011-2018)

- "Nonadiabatic Molecular Dynamics For Electron and Energy Transfer: Applications to Artificial Photosynthesis" (2011-2014)
- Presidential Early Career Award for Science and Engineering (PECASE): (2013-2018)

7. Invited Talks

- June, 2016: Excited State Processes, LANL, New Mexico
- June, 2016: Telluride Conference on Quantum Dynamics, Telluride, CO
- June, 2016: CECAM: Molecular Quantum Dynamics, Lausanne, Switzerland
- May, 2016: Air Force Office of Scientific Research Contractor's Meeting, Washington, DC
- May, 2016: Ki-Net: Mathematical and Computational Methods in Quantum Chemistry, Yale University
- March, 2016: APS March Meeting, DCP/JCP Highlights, Baltimore, MD
- August, 2015: American Chemical Society, Journal of Physical Chemistry Lectureship, Boston, MA
- July, 2015: Telluride Conference on Quantum Dynamics, Telluride, CO
- July, 2015: Dynamics of Molecular Collisions, Asilomar, CA
- June, 2015: CECAM, Quantum Dynamics workshop, Lausanne, Switzerland
- June, 2015: The Batsheva de Rothschild Seminar on Molecular Electronics 2015, Israel
- March, 2015: University of Karlsruhe
- March, 2015: EPFL, Lausanne
- March, 2015: ETH, Zurich
- February, 2015: University of Houston
- February, 2015: Rice University
- November, 2014: University of Colorado
- October, 2014: CUNY Workshop
- September, 2014: Duke University

- July, 2014: Gordon Research Conference, Atomic and Molecular Interactions.
- June, 2014: Telluride Conference, Quantum Dynamics in the Condensed Phase.
- June, 2014: University of Washington
- May, 2014: Contractor's Meeting, Washington DC, Air Force Office of Scientific Research
- May, 2014: 2014 Workshop on Dynamical Quantum Effects in Molecular Processes, CUNY
- May, 2014: University of CA, Irvine
- March, 2014: Penn State University
- February, 2014: University of CA, San Diego
- February, 2014: Harvard University
- January, 2014: University of Toronto
- December, 2013: Haverford University
- November, 2013: CECAM Conference, "Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality," Israel
- November, 2013: Stanford University
- November, 2013: University of California, Berkeley
- October, 2013: Excited States and Complex Environments, ESCE2013, Münster, Germany
- October, 2013: Johns Hopkins University
- October, 2013: University of Illinois
- September, 2013: Boston University.
- September, 2013: Columbia University.
- Summer 2013: Gordon Research Conference on Time Dependent Density Functional Theory, MA
- July, 2013: Quantum effects in condensed-phase systems, Telluride, CO.
- June, 2013: New Frontiers in Electron Correlation, Telluride, CO.
- May, 2013: University of Wisconsin
- April, 2013: Tulane University
- March, 2013: ANSER (Argonne-Northwestern Solar Energy Research Center)
- February, 2013: Lawrence-Livermore National Laboratory
- January, 2013: Wayne-State University
- November 2012: University of Chicago.
- June 2012: Condensed Phase Dynamics, Telluride, CO.
- April, 2012: University of Oregon
- March 2012: American Chemical Society, Symposium on Surface Hopping. San Diego, CA.
- March, 2012: University of Utah
- February 2012: Ohio-State University
- January 2012, University of California, Berkeley
- November 2011: City University of New York (CUNY), Initiative for the Theoretical Sciences at the Graduate Center.
- August 2011: American Chemical Society, Session on Reduced Density Matrices. Denver, CO.

- July 2011: MERCURY: Molecular Education and Research Consortium in Undergraduate computational Chemistry. Bucknell University, PA
- July 2011: American Conference in Theoretical Chemistry. Telluride, CO
- July 2011: Conference on Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy. Telluride, CO
- October 8, 2010: Rutgers-Newark University, NJ
- July 18, 2010: Condensed Phase Dynamics, Telluride, CO.
- July 1, 2010: NIH, theory seminar
- June 5, 2010: Electronic Structure 10 Conference, Austin, TX
- January 29, 2009. University of Colorado, Boulder, Physical Chemistry Seminar.
- January 20, 2009. University of Chicago , Physical Chemistry Seminar.
- January 8, 2009. Yale University, Physical Chemistry Seminar.
- December 4, 2008. University of Pennsylvania, Physical Chemistry Seminar.
- December 17, 2007. Eilat, Israel. The Gentner-Minerva Symposium on Time-Dependent Density Functional Theory.
- September 1 2007. Lyon, France, CECAM (Centre Européen de Calcul Atomique et Moléculaire).
- January 24, 2007. Columbia University, Physical Chemistry Seminar.
- January 11, 2007. UCLA, Physical Chemistry Seminar.

8. Contributed Talks:

- July 2012. Gordon Research Conference on *Atomic and Molecular Interactions*.
- March 2011. American Chemical Society, Tunneling Pathways Symposium.
- March 7, 2007. Denver, American Physical Society.
- September 10, 2006. San Francisco, American Chemical Society, Physical Division. Symposia: Frontiers in Molecular Biophysical Dynamics: Experiment and Theory.
- September 1, 2005. Washington D.C. American Chemical Society, Physical Division. Symposia: Computational Exploration of Energy Landscapes: Challenges and Solutions.

9. Teaching Experience

Graduate Quantum Mechanics I
Honors Freshman Chemistry II

10. Languages Spoken

Hebrew and French (fluently), Spanish (comfortably)

11. Professional Service

- Co-organizer, Penn Conference in Theoretical Chemistry (August, 2016)
- Organizer, NSF Workshop in Wavepacket dynamics (July, 2016)
- Co-organizer, Penn Conference in Theoretical Chemistry (August, 2015)
- Organizer, NSF/Q-Chem Workshop in Electronic Structure Theory at the MERCURY undergraduate symposium in quantum chemistry (July, 2013)
- Organizer, "Q-Chem 2012 developer meeting" (August, 2012)

- Co-organizer, Symposium on "Electron and Energy Transfer Phenomena: At the Intersection of Electronic Structure Theory and Chemical Dynamics", National Meeting of the American Chemical Society (Fall, 2012)
- Co-organizer, "Electronic Structure '11" Conference in Condensed Matter Physics, University of Pennsylvania, (June, 2011)

12. Editorial Positions:

Reviewer: *Journal of Chemical Physics*
Journal of Physical Chemistry
Chemical Physics
Molecular Physics
Proceedings of the National Academy of Science
Nature, Nature Communications
Journal of Chemical Theory and Computation
Physical Chemistry Chemical Physics

National Science Foundation
Department of Energy
Department of Defense

13. Publications (all in refereed journals):

Available at http://subotnikgroup.chem.upenn.edu/publications.html

Independent Publications (University of Pennsylvania):

67. J. E. Subotnik, A. Jain, B. Landry, A. Petit, W. Ouyang and N. Bellonzi. "Understanding The Surface Hopping View of Electronic Transitions and Decoherence"
Ann. Rev. Phys. Chem., **67**, 387-417 (2016)

66. N. Bellonzi, A. Jain and J. E. Subotnik. "An assessment of mean-field mixed semiclassical approaches: equilibrium populations and algorithm stability"
J. Chem. Phys. **144**, 154110 (2016) link

65. W. Dou, A. Nitzan, and J.E. Subotnik. "Molecular electronic states near metal surfaces at equilibrium using potential of mean force and numerical renormalization group methods: Hysteresis revisited."
J. Chem. Phys. **144**, 074109 (2016) link

64. W. Dou and J. E. Subotnik. A broadened classical master equation approach for nonadiabatic dynamics at metal surfaces: Beyond the weak molecule-metal coupling limit.
J. Chem. Phys. **144**, 024116 (2016) link

63. A. Jain and J. E. Subotnik. "Does Nonadiabatic Transition State Theory Make Sense Without Decoherence?"
J. Phys. Chem. Lett. **6**, 4809-4814 (2015) link

62. A. Jain and J.E. Subotnik. "Surface hopping, transition state theory and decoherence II: Thermal rate constants and detailed balance."
J. Chem. Phys. **143**, 134107 (2015) link

61. A. Jain, M. F. Herman, W. Ouyang and J. E. Subotnik "Surface hopping, transition state theory and decoherence I: Scattering theory and time-reversibility."
J. Chem. Phys. **143**, 134106 (2015) link

60. W. Ouyang, J. Saven, and J. E. Subotnik. "A Surface Hopping View of Electrochemistry: Non-Equilibrium Electronic Transport through an Ionic Solution with a Classical Master Equation"
J. Phys. Chem. C., **119,** 20833-20844 (2015) link

59. A. S. Petit and J.E. Subotnik. "Appraisal of Surface Hopping as a Tool for Modeling Condensed Phase Linear Absorption Spectra."
J. Chem. Theor. Comp., **11**, 4328-4341 (2015) link

58. W. Dou, A. Nitzan, and J.E. Subotnik. "Frictional effects near a metal surface."
J. Chem. Phys., **143**, 054103 (2015) link

57. W. Dou, A. Nitzan, and J.E. Subotnik. " Surface hopping with a manifold of electronic states. III. Transients, broadening, and the Marcus picture."
J. Chem. Phys., **142**, 234106 (2015) link

56. J. E. Subotnik, E. C. Alguire, Q. Ou, B. R. Landry, S. Fatehi. "The Requisite Electronic Structure Theory To Describe Photoexcited Nonadiabatic Dynamics: Nonadiabatic Derivative Couplings and Diabatic Electronic Couplings"
Acc. Chem. Res. **48**, 1340-1350 (2015) link

55. B. R. Landry and J. E. Subotnik. "Surface hopping outperforms secular Redfield theory when reorganization energies range from small to moderate (and nuclei are classical)"
J. Chem. Phys., **142**, 104102 (2015) link

54. W. Dou, A. Nitzan, and J.E. Subotnik "Surface hopping with a manifold of electronic states. II. Application to the many- body Anderson-Holstein model"
J. Chem. Phys., **142**, 084110 (2015) link

53. W. Ouyang, W. Dou, and J. E. Subotnik. "Surface hopping with a manifold of electronic states. I. Incorporating surface-leaking to capture lifetimes."
J. Chem. Phys., **142**, 084109 (2015) link

52. Q. Ou, G. Bellchambers, F. Furche, and J. E. Subotnik, "First-order derivative couplings between excited states from adiabatic TDDFT response theory."
*J. Chem. Phys.,***142**, 064114 (2015) link
*JCP Editors' Choice (2015)

51. J. E. Subotnik and Y. M. Rhee, "On Surface Hopping and Time-Reversal."
J. Phys. Chem. A., **119**, 990-995 (2015) link

50. E. Alguire, J. E. Subotnik, N. Damrauer, "Exploring Non-Condon Effects in a Covalent Tetracene Dimer: How Important Are Vibrations in Determining the Electronic Coupling for Singlet Fission?"
*J. Phys. Chem. A.,***119**, 299-311 (2015) link

49. B. Veldkamp, X. Liu, M. Wasielewski, J. E. Subotnik and M. A. Ratner, "Molecular Excited States: Accurate Calculation of Relative Energies and Electronic Coupling Between Charge Transfer and Non-Charge Transfer States."
*J. Phys. Chem. A.,***119**, 253-262 (2015) link

48. Y. Shao, *et al.* "Advances in molecular quantum chemistry contained in the Q-Chem 4 program package."
Mol. Phys. **113**, 184-215 (2015) link

47. A. S. Petit and J. E. Subotnik. "Calculating time-resolved differential absorbance spectra for ultrafast pump-probe experiments with surface hopping trajectories."
J. Chem. Phys. **141**, 154108 (2014) link

46. B. R. Landry and J. E. Subotnik. "Quantifying the Lifetime of Triplet Energy Transfer Processes in Organic Chromophores: A Case Study of 4‑ (2-Naphthylmethyl)benzaldehyde."
J. Chem. Theory. Comp., **10**, 4253 (2014) link

45. K. Samanta, J. Beames, M. Lester and J. E. Subotnik. "Quantum dynamical investigation of the simplest Criegee intermediate CH2OO and its O–O photodissociation channels."
J. Chem. Phys., **141**, 134303 (2014) link

44. E. Alguire, Q. Ou., and J. E. Subotnik "Calculating Derivative Couplings between TDHF Excited States with Pseudo-Wavefunctions",
J. Phys. Chem. B. **119**, 7140-7149 (2015) link

43. Q. Ou., E. Alguire, and J. E. Subotnik " Derivative Couplings between TD-DFT Excited States in the Random-Phase Approximation Based on Pseudo-Wavefunctions: Behavior around Conical Intersections",
J. Phys. Chem. B. **119**, 7150-7161 (2015) link

42. Q. Ou, S. Fatehi, E. Alguire, Y. Shao and J. E. Subotnik. "Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation." *J. Chem. Phys.* **141**, 024114 (2014) link

41. A. Petit and J. E. Subotnik. "How to calculate linear absorption spectra with lifetime broadening using fewest switches surface hopping trajectories: A simple generalization of ground-state Kubo theory." *J. Chem. Phys*, **141**, 014107 (2014) link

40. Ouyang and Subotnik. "Estimating the entropy and quantifying the impurity of a swarm of surface-hopping trajectories: A new perspective on decoherence."
J. Chem. Phys. **140**, 204102 (2014) link
*JCP Editors' Choice (2014)

39. Falk, Landry and Subotnik. "Can Surface Hopping sans Decoherence Recover Marcus Theory? Understanding the Role of Friction in a Surface Hopping View of Electron Transfer."
J. Phys. Chem. B, **118,** 8108-8117 (2014) link

38. X. Liu and J. E. Subotnik, "The variationally orbital-adapted configuration interaction singles (VOA-CIS) approach to electronically excited states,"
J. Chem. Theory Comp. **10**, 1004-1020 (2014) link

37. E. C. Alguire, S. Fatehi, Y. Shao, and J. E. Subotnik, "Analysis of localized diabatic states beyond the condon approximation for excitation energy transfer processes,"
J. Phys. Chem. A, **118**, 11891–11900 (2014) link

36. B. R. Landry, M. J. Falk, and J. E. Subotnik. "The correct interpretation of surface hopping trajectories: How to calculate electronic properties"
J. Chem. Phys. (Communications) **139**, 211101 (2013) link

35. J. E. Subotnik, W. Ouyang, and B. R. Landry. "Can We Derive Tully's Surface-Hopping Algorithm from the Semiclassical Quantum Liouville Equation? Almost, but only with Decoherence"
J. Chem. Phys. **139**, 214107 (2013) link

34. Q. Ou and J. E. Subotnik. "Electronic Relaxation in Benzaldehyde evaluated via TD-DFT and Localized Diabatization: Intersystem Crossings, Conical Intersections, and Phosphorescence" *J. Phys. Chem. C.,* **117**, 19839-19849 (2013) link

33. S. Fatehi, E. Alguire, and J. E. Subotnik. "Derivative couplings and analytic gradients for diabatic states, with an implementation for Boys-localized configuration-interaction singles"
J. Chem. Phys., **139**, 124112 (2013) link

32. X. Liu, Q. Ou, E. Alguire and J. E. Subotnik. "An Inexpensive, Variational, Almost Black-Box, Almost Size-Consistent, Correction to Configuration Interaction Singles for Valence Excited States."
J. Chem. Phys. (Communication), **138**, 221105 (2013) link
**(JCP top 20 downloaded, June, 2013)*

31. E. Alguire and J. E. Subotnik. "Optimal diabatic states based on solvation parameters."
J. Chem. Phys., **137**, 194108 (2012) link

30. B. Landry and J. E. Subotnik. "How to recover Marcus theory with fewest switches surface hopping: Add just a touch of decoherence."
J. Chem. Phys. **137**, 22A513 (2012) link

29. S. Fatehi and Subotnik. "Derivative Couplings with Built-In Electron-Translation Factors: Application to Benzene."
J. Phys. Chem. Lett., **3**, 2039 (2012) link

28. X. Liu, S. Fatehi, Y. Shao, B. Veldkamp, J. E. Subotnik "Communication: Adjusting charge transfer state energies for configuration interaction singles: Without any parameterization and with minimal cost."
J. Chem. Phys. **136**, 161101 (2012) link

27. B. Landry and J. E. Subotnik "Standard Surface Hopping Predicts Incorrect Scaling for Marcus' Golden-Rule Rate: The Decoherence Problem Cannot Be Ignored."
J. Chem. Phys. (Communications) **135**, 191101 (2011) link
**(JCP top 20 downloaded, November, 2011; JCP Editor's Choice, 2011)*

26. S. Fatehi, E. Alguire, Y. Shao and J. E. Subotnik "Analytical derivative couplings between configuration-interaction-singles states with built-in electron translation factors for translational invariance."
J. Chem. Phys. **135**, 234105 (2011) link

25. J. E. Subotnik "Fewest Switches Surface Hopping and Decoherence in Multiple Dimensions." *J. Phys. Chem. A.* **115**, 12083 (2011) link

24. J. E. Subotnik "Configuration Interaction Singles Has a Large Systematic Bias Against Charge-Transfer States."
J. Chem. Phys. (Communications) **135,** 071104 (2011) link
**(JCP top 20 downloaded, August, 2011)*

23. E. Alguire and J. E. Subotnik. "Diabatic couplings for charge recombination via Boys localization and spin-flip configuration interaction singles."
J. Chem. Phys. **135,** 044114 (2011) link

22. N. Shenvi, J. E. Subotnik and W. T. Yang. "Phase-corrected surface hopping: Correcting the phase evolution of the electronic wavefunction."
J. Chem. Phys. **135,** 024101 (2011) link
**(JCP top 20 downloaded, July, 2011)*

21. J. E. Subotnik and N. Shenvi. Decoherence and surface hopping: "When can averaging over initial conditions help capture the effects of wave packet separation?"
J. Chem. Phys. **134,** 244114 (2011) link

20. N. Shenvi, J. E. Subotnik , and W. Yang. "Simultaneous-trajectory surface hopping: a parameter-free algorithm for implementing decoherence in nonadiabatic dynamics."

J. Chem. Phys. **134**, *144102 (2011)* link

19. J. E. Subotnik and N. Shenvi "A New Approach to Decoherence and Momentum Rescaling in the Surface Hopping Algorithm."
J. Chem. Phys. **134**, 024105 (2011) link

18. J. Vura-Weis, M. D. Newton, M. Wasielewski, and J. E. Subotnik "Characterizing the Locality of Diabatic States for Electronic Excitation Transfer By Decomposing the Diabatic Coupling."
J. Phys. Chem. C , **114**, 20449 (2010) link

17. J. E. Subotnik. "Augmented Ehrefenst Dynamics Yields a Rate for Surface Hopping."
J. Chem. Phys. **132**, 134112 (2010) link

Postdoctoral Publications:

16. C. Hermann, G. C. Solomon, J. E. Subotnik, V. Mujica and M. A. Ratner. "Ghost Transmission: How large basis sets can make electron transport calculations worse."
J. Chem. Phys. 132, 024103 (2010) link

15. J. E. Subotnik, J. Vura-Weis, A. Sodt, and M. A. Ratner. "Predicting Accurate Electronic Excitation Transfer Rates via Marcus Theory with Boys or Edmiston-Ruedenberg Localized Diabatization."
J. Phys. Chem. A. **114**, 8665 (2010) link

14. J. E. Subotnik, R. J. Cave, R. P. Steele and N. Shenvi. "The Initial and Final States of Electron and Energy Transfer Processes: Diabatization According to System-Solvent Interactions."
J. Chem. Phys. **130**, 234102 (2009) link

13. J. E. Subotnik, T. Hansen, M. A. Ratner and A. Nitzan. "Nonequilibrium Steady State Transport via the Reduced Density Matrix Operator."
J. Chem. Phys. **130**, 144105 (2009) link

12. J. E. Subotnik, S. Yeganeh, R. J. Cave, and M. A. Ratner. "Constructing Diabatic States from Adiabatic States: Extending Generalized Mulliken-Hush to Multiple Charge Centers with Boys Localization."
J. Chem. Phys. **129**, 244101 (2008) link

11. J. E. Subotnik and A. Nitzan. "Multibody Scattering, Correlation, Molecular Conduction and the 0.7 Anomaly."
J. Chem. Phys. **129,** 144107 (2008) link

Publications from Graduate School:

10. J. E. Subotnik and M. Head-Gordon. "Exploring The Accuracy of Relative Molecular Energies With Local Correlation Theory."
J. Phys: Cond. Matter, **20,** 294211 (2008) link

9. J. E. Subotnik, A. Sodt and M. Head-Gordon. "The Limits of Local Correlation Theory: Electronic Delocalization and Chemically Smooth Potential Energy Surfaces." *J. Chem. Phys.* **128,** 034103 (2008) link

8. J. E. Subotnik, A. Sodt and M. Head-Gordon. "Localized Orbital Theory and Ammonia Triborane." *Phys. Chem. Chem. Phys,* **9,** 5522 (2007) link

7. A. Sodt, J. E. Subotnik, and M. Head-Gordon "Linear Scaling Density Fitting." *J. Chem. Phys.* **125**, 194109 (2006) link

6. J. E. Subotnik, A. Sodt, and M. Head-Gordon. "A Near Linear Scaling Smooth Coupled Cluster Algorithm For Electronic Structure." *J. Chem. Phys*. **125**, 074116 (2006) link

5. Y. Shao, *et al.* "Advances in methods and algorithms in a modern quantum chemistry program package." *Phys. Chem. Chem. Phys.* **8,** 3172 (2006) link

4. J. E. Subotnik, A. D. Dutoi and M. Head-Gordon. "Fast localized orthonormal virtual orbitals that depend smoothly on nuclear coordinates." *J. Chem. Phys.* **123**, 114108 (2005) link

3. J.E. Subotnik, M. Head-Gordon. "A local correlation model that yields intrinsically smooth potential-energy surfaces." *J. Chem. Phys.* **123,** 064108 (2005) link

2. J. E. Subotnik, M. Head-Gordon. "A localized basis that allows fast and accurate second order Moller Plesset calculations." *J. Chem. Phys.* **122**, 034109 (2005) link

1. J.E. Subotnik, Y.Shao, W. Liang, and M. Head-Gordon. "An efficient method for calculating maxima of homogenous functions of orthogonal matrices. Applications to localized occupied orbitals." *J. Chem. Phys.* **121**, 9220 (2004) link

14. Students Supervised:

Undergraduate:

Martin Falk (NSF and DOD graduate fellowship at MIT)
Razzi Abuissa

Postdoctoral Fellows:

Amber Jain (current)
Greg Medders (current)

Kousik Samanta (assistant professor at IIT Bhubaneswar, India)
Shervin Fatehi (assistant professor at University of Texax, Rio Grande Valley)
Brian Landry

Graduate Students:
Qi Ou (current)
Wenjun Ouyang (current)
Wenjie Dou (current)
Nicole Bellonzi (current)
Zuxin Jin (current)
Gaohan Mao (current)

Xinle Liu (JP Morgan)
Ethan Alguire (Schrodinger)

15. University Service
Faculty Senate Executive Committee (2015 - 2018)
Phi Beta Kappa Electoral Board Member (2016 - 2019)

16. Departmental Service
Graduate Admissions Committee (2010-2015)
Physical Chemistry Seminar Commitee (2010 - present)
Donner Chair Search Committee (2013- present) ; chair (2015 - present)