

Curriculum Vitae
Joseph Eli Subotnik

October, 2017.

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.
- September 2016 - June 2017 Visiting Associate Professor, Stanford University and SLAC National Accelerator Laboratory, PULSE Institute
- 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

- August, 2017, World Association of Theoretically Oriented Chemistry (WATOC), Munich, Germany
- July, 2017, Telluride Conference in Quantum Transport
- July, 2017, Telluride Conference in Quantum Dynamics
- July, 2017, American Conference in Theoretical Chemistry, Boston, MA
- May, 2017, Canadian Society for Chemistry Conference, Toronto, Canada
- April, 2017, American Chemical Society, San Francisco, CA
- February, 2017 University of Southern California
- Virtual Winter Summer School, <https://winterschool.cc/>
- September, 2016 University of the Pacific, CA
- 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

- Organizer, Penn Conference in Theoretical Chemistry (2015 – present)
- Organizer, NSF Tutorial in Wavepacket dynamics at the MERCURY undergraduate symposium in quantum chemistry (July, 2016)
- 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):

79. W. Dou and J. E. Subotnik. "Universality of electronic friction: Equivalence of von Oppen's nonequilibrium Green's function approach and the Head-Gordon-Tully model at equilibrium "
Phys. Rev. B. **96**, 104305 (2017)
<http://dx.doi.org/10.1103/PhysRevB.96.104305>
78. Tianyi Liu, Annemarie L. Exarhos, Ethan C. Alguire, Feng Gao, Elmira Salami-Ranjbaran, Kevin Cheng, Tiezheng Jia, Joseph E. Subotnik, Patrick J. Walsh, James M. Kikkawa, and

Zahra Fakhraei "Birefringent Stable Glass with Predominantly Isotropic Molecular Orientation"

Phys. Rev. Lett. **119**, 095502 (2017)

<http://dx.doi.org/10.1103/PhysRevLett.119.095502>

77. W. Dou, G. Miao, and J. E. Subotnik. "Born-Oppenheimer Dynamics, Electronic Friction, and the Inclusion of Electron-Electron Interactions"

Phys. Rev. Lett., **119**, 046001 (2017)

<http://dx.doi.org/10.1103/PhysRevLett.119.046001>

76. Z. Jin and J. E. Subotnik. "Localized diabaticization applied to excitons in molecular crystals"

J. Chem. Phys. **146**, 244110 (2017)

<http://dx.doi.org/10.1063/1.4986952>

75. W. Dou and J. E. Subotnik. "A Generalized Surface Hopping Algorithm To Model Nonadiabatic Dynamics near Metal Surfaces: The Case of Multiple Electronic Orbitals"

J. Chem. Theor. Comp. **13**, 2430-2439 (2017)

<http://dx.doi.org/10.1021/acs.jctc.7b00094>

74. G. Medders, E. Alguire, A. Jain, and J. E. Subotnik. "Ultrafast Electronic Relaxation through a Conical Intersection: Nonadiabatic Dynamics Disentangled through an Oscillator Strength-Based Diabatization Framework"

J. Phys. Chem. A **121**, 1425-1434 (2017)

<http://dx.doi.org/10.1021/acs.jpca.6b12120>

73. D. B. Straus, S. H. Parra, N. Iotov, J. Gebhardt, A. M. Rappe, J. E. Subotnik, J. M. Kikkawa, and C. R. Kagan. "Direct Observation of Electron-Phonon Coupling and Slow Vibrational Relaxation in Organic-Inorganic Hybrid Perovskites"

JACS Comm. **138**, 13798-13801 (2016)

<http://dx.doi.org/10.1021/jacs.6b08175>

72. A. Jain, E. Alguire, and J. E. Subotnik. "An Efficient, Augmented Surface Hopping Algorithm That Includes Decoherence for Use in Large-Scale Simulations"

J. Chem. Theory Comp., **12**, 5256-5268 (2016)

<http://dx.doi.org/10.1021/acs.jctc.6b00673>

71. W. Ouyang, W. Dou, A. Jain and J.E. Subotnik. "Dynamics of Barrier Crossings for the Generalized Anderson Holstein Model: Beyond Electronic Friction and Conventional Surface Hopping"

J. Chem. Theor. Comp. **12**, 4178-4183 (2016)

<http://dx.doi.org/10.1021/acs.jctc.6b00533>

70. W. Dou and J.E. Subotnik. "A many-body states picture of electronic friction: The case of multiple orbitals and multiple electronic states."

J. Chem. Phys. **145**, 054102 (2016)

<http://dx.doi.org/10.1063/1.4959604>

69. W. Dou and J.E. Subotnik. "Electronic friction near metal surfaces: a case where molecule-metal couplings depend on nuclear coordinates."
J. Chem. Phys. (accepted) (2016)
<https://arxiv.org/abs/1606.06110>
68. Q. Ou and J.E. Subotnik. "Comparison between GW and Wave-Function-Based Approaches: Calculating the Ionization Potential and Electron Affinity for 1D Hubbard Chains."
J. Phys. Chem. A. **120**, 4514-4525 (2016)
<http://dx.doi.org/10.1021/acs.jpca.6b03294>
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)
<http://dx.doi.org/10.1146/annurev-physchem-040215-112245>
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)
<http://dx.doi.org/10.1063/1.4946810>
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)
<http://dx.doi.org/10.1063/1.4941848>
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)
<http://dx.doi.org/10.1063/1.4939734>
63. A. Jain and J. E. Subotnik. "Does Nonadiabatic Transition State Theory Make Sense Without Decoherence?"
J. Phys. Chem. Lett. **6**, 4809-4814 (2015)
<http://dx.doi.org/10.1021/acs.jpcelett.5b02148>
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)
<http://dx.doi.org/10.1063/1.4930549>
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)
<http://dx.doi.org/10.1063/1.4930548>
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)
<http://dx.doi.org/10.1021/acs.jpcc.5b06655>
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)
<http://dx.doi.org/10.1021/acs.jctc.5b00510>
58. W. Dou, A. Nitzan, and J.E. Subotnik. "Frictional effects near a metal surface."
J. Chem. Phys., **143**, 054103 (2015)
<http://dx.doi.org/10.1063/1.4927237>
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)
<http://dx.doi.org/10.1063/1.4922513>
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)
<http://dx.doi.org/10.1021/acs.accounts.5b00026>
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)
<http://dx.doi.org/10.1063/1.4913494>
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)
<http://dx.doi.org/10.1063/1.4908034>
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)
<http://dx.doi.org/10.1063/1.4908032>
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)
*JCP Editors' Choice (2015)
<http://dx.doi.org/10.1063/1.4906941>
51. J. E. Subotnik and Y. M. Rhee, "On Surface Hopping and Time-Reversal."
J. Phys. Chem. A., **119**, 990-995 (2015)
<http://dx.doi.org/10.1021/jp512024w>
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)
<http://dx.doi.org/10.1021/jp510777c>
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)
<http://dx.doi.org/10.1021/jp508337x>
48. Y. Shao, *et al.* "Advances in molecular quantum chemistry contained in the Q-Chem 4 program package."
Mol. Phys. **113**, 184-215 (2015)
<http://dx.doi.org/10.1080/00268976.2014.952696>
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)
<http://dx.doi.org/10.1063/1.4897258>
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)
<http://dx.doi.org/10.1021/ct500583d>
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)
<http://dx.doi.org/10.1063/1.4894746>
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)
<http://dx.doi.org/10.1021/jp5057682>

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)
<http://dx.doi.org/10.1021/jp505767b>
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)
<http://dx.doi.org/10.1063/1.4887256>
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)
<http://dx.doi.org/10.1063/1.4884945>
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)
*JCP Editors' Choice (2014)
<http://dx.doi.org/10.1063/1.4876491>
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)
<http://dx.doi.org/10.1021/jp5011346>
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)
<http://dx.doi.org/10.1021/ct4009377>
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)
<http://dx.doi.org/10.1021/jp411107k>
36. B. R. Landry, M. J. Falk, and J. E. Subotnik. "Communication: The correct interpretation of surface hopping trajectories: How to calculate electronic properties"
J. Chem. Phys. **139**, 211101 (2013)
<http://dx.doi.org/10.1063/1.4837795>
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)
<http://dx.doi.org/10.1063/1.4829856>
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)
<http://dx.doi.org/10.1021/jp405574q>
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)
<http://dx.doi.org/10.1063/1.4820485>
32. X. Liu, Q. Ou, E. Alguire and J. E. Subotnik. "Communication: An Inexpensive, Variational, Almost Black-Box, Almost Size-Consistent, Correction to Configuration Interaction Singles for Valence Excited States."
J. Chem. Phys., **138**, 221105 (2013)
*(*JCP* top 20 downloaded, June, 2013)
<http://dx.doi.org/10.1063/1.4809571>
31. E. Alguire and J. E. Subotnik. "Optimal diabatic states based on solvation parameters."
J. Chem. Phys., **137**, 194108 (2012)
<http://dx.doi.org/10.1063/1.4766463>
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)
<http://dx.doi.org/10.1063/1.4733675>
29. S. Fatehi and Subotnik. "Derivative Couplings with Built-In Electron-Translation Factors: Application to Benzene."
J. Phys. Chem. Lett., **3**, 2039 (2012)
<http://dx.doi.org/10.1021/jz3006173>
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)
<http://dx.doi.org/10.1063/1.47505757>
27. B. Landry and J. E. Subotnik "Communication: Standard Surface Hopping Predicts Incorrect Scaling for Marcus' Golden-Rule Rate: The Decoherence Problem Cannot Be Ignored."
J. Chem. Phys. **135**, 191101 (2011)
*(*JCP* top 20 downloaded, November, 2011; *JCP* Editor's Choice, 2011)
<http://dx.doi.org/10.1063/1.3663870>

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)
<http://dx.doi.org/10.1063/1.3665031>
25. J. E. Subotnik "Fewest Switches Surface Hopping and Decoherence in Multiple Dimensions." *J. Phys. Chem. A.* **115**, 12083-12096 (2011)
<http://dx.doi.org/10.1021/jp206557h>
24. J. E. Subotnik "Communication: Configuration Interaction Singles Has a Large Systematic Bias Against Charge-Transfer States."
J. Chem. Phys. **135**, 071104 (2011)
*(JCP top 20 downloaded, August, 2011)
<http://dx.doi.org/10.1063/1.3627152>
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)
<http://dx.doi.org/10.1063/1.3615493>
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)
*(JCP top 20 downloaded, July, 2011)
<http://dx.doi.org/10.1063/1.3603447>
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)
<http://dx.doi.org/10.1063/1.3603448>
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)
<http://dx.doi.org/10.1063/1.3575588>
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)
<http://dx.doi.org/10.1063/1.3506779>
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)
<http://dx.doi.org/10.1021/jp104783r>

17. J. E. Subotnik. “Augmented Ehrenfest Dynamics Yields a Rate for Surface Hopping.”
J. Chem. Phys. **132**, 134112 (2010)
<http://dx.doi.org/10.1063/1.3314248>

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.”
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14. Students Supervised:

Undergraduate:

Martin Falk (NSF and DOD graduate fellowship at MIT)

Razzi Abuissa (professional programmer)

Gideon Haber (current)

Postdoctoral Fellows:

Amber Jain (current)

Greg Medders (current)

Hsing-Ta Chen (current)

Kousik Samanta (assistant professor at IIT Bhubaneswar, India)

Shervin Fatehi (assistant professor at University of Texas, Rio Grande Valley)

Brian Landry

Graduate Students:

Wenjie Dou (current)

Nicole Bellonzi (current)

Zuxin Jin (current)

Gaohan Mao (current)

Tao Li (current)

Alec Coffman (current)

Xinle Liu (MTV)

Ethan Alguire (Schrodinger Inc.)

Qi Ou (postdoc at Princeton)

Wenjun Ouyang (Susquehanna Bank)

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 Committee (2010 - 2016)

Donner Chair Search Committee (2013- present) ; chair (2015 - 2016)