Benjamin G. Levine

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Education

University of Illinois at Urbana-Champaign, Urbana, IL **2001-2007**
Ph.D. in Chemistry
Graduate Adviser: Todd J. Martínez
Dissertation: Nonadiabatic dynamics of *cis-trans* photoisomerization – a first principles study

University of Illinois at Urbana-Champaign, Urbana, IL **1997-2001**
B.S. in Chemical Engineering

Experience

IACS Endowed Chair of Chemistry, Institute for Advanced Computational Science and Dept. of Chemistry, Stony Brook University **2020-present**
Affiliate Professor, Department of Physics, Stony Brook University **2024-present**
Adjunct Assistant Professor, Department of Chemistry, Michigan State University **2020-2021**
Associate Professor, Department of Chemistry, Michigan State University **2017-2020**
Assistant Professor, Department of Chemistry, Michigan State University **2011-2017**
Postdoctoral Research Assistant, Temple University **2009-2011**
Supervised by Professor Michael L. Klein
Postdoctoral Research Assistant, University of Pennsylvania **2007-2009**
Supervised by Professor Michael L. Klein

Awards and Honors

- 2017 JPCA/PHYS Lectureship (from the ACS PHYS division and Journal of Physical Chemistry)
- Spring 2017 OpenEye Outstanding Junior Faculty Award in Computational Chemistry (from the ACS COMP division)

Current Funding

10/2023-3/2025 Predicting Structure-Property Relationships in Optoelectronic Materials, NSF ACCESS, CHE140101, 1,500,000 ACCESS credits (units of computer time; approx. value $18,000), PI: Levine

9/2023-8/2026	Light Harvesting in Semiconductor Quantum Dots, DE-SC0021197, DOE BES, $909,000, PI: Warren Beck (MSU), co-PIs: Levine, Gregory Van Patten (Middle Tennessee State)
11/2022-6/2026	Definitive Simulation of Photodynamics on Many Electronic States, DOE BES, DE-SC0021643, $450,000, PI: Levine
7/2021-6/2024	Collaborative Research: Understanding Ultrafast Observables, NSF, CHE-2102319, $675,000, PI: Thomas Allison (SBU), co-PIs: Levine, Thomas Weinacht (SBU)

Past Funding

8/2020-7/2024	First Principles Simulation Methods for Strong Field Dynamics, NSF, CHE1954519, $480,000, PI: Levine
10/2022-9/2023	Predicting Structure-Property Relationships in Optoelectronic Materials, NSF ACCESS (formerly XSEDE), CHE140101, 16,000 GPU hrs, PI: Levine
9/2020-8/2023	Light Harvesting in Semiconductor Quantum Dots, DE-SC0021197, DOE BES, $600,000, PI: Warren Beck (MSU), co-PIs: Levine, Gregory Van Patten (Middle Tennessee State)
8/2018-7/2022	QLC: EAGER: Quantum control of energy transfer pathways and chemical reactions, NSF, CHE-1836498, $294,287, PI: Marcos Dantus (MSU), co-PI: Levine
10/2021-9/2022	Predicting Structure-Property Relationships in Optoelectronic Materials, NSF XSEDE, CHE140101, 40,400 GPU hrs, PI: Levine
5/2021-10/2022	A Multireference Approach to Electron and Electron-Nuclear Dynamics in Nanomaterials, DOE BES, DE-SC0021643, $64,589, PI: Levine (Note: this is the remainder of DE-SC0018432 transferred to Stony Brook)
10/2020-9/2021	Predicting Structure-Property Relationships in Optoelectronic Materials, NSF XSEDE, CHE140101, Computer time valued $3,647, PI: Levine
6/2018-8/2020	A Multireference Approach to Electron and Electron-Nuclear Dynamics in Nanomaterials, DOE BES, DE-SC0018432, $325,000, PI: Levine
10/2017-9/2020	Ab Initio Molecular Dynamics above the Ionization Threshold, AFOSR, FA9550-17-1-0411, $343,883, PI: Levine

4/2019-9/2020	Predicting Structure-Property Relationships in Optoelectronic Materials, NSF XSEDE, CHE140101, Computer time valued $9,422.00, PI: Levine
5/2016-4/2020	Accurate Nonadiabatic Dynamics at Conical Intersections in Nanomaterials, NSF, CHE-1565634, $405,001, PI: Levine
5/2018	A Multireference Approach to Electron and Electron-Nuclear Dynamics in Nanomaterials, NVidia Professor Partnership, computer hardware valued ~$1,200, PI: Levine
4/2018-3/2019	Predicting Structure-Property Relationships in Optoelectronic Materials, NSF XSEDE, CHE140101, Computer time valued $3,797.53, PI: Levine
7/2015-6/2018	Displacing Fossil Fuels with Multi-Junction Perovskite Photovoltaics, MSU Strategic Partnership Grant, $399,996, PI: Hamann, co-PIs: Duxbury, Levine, Lunt, McCusker, Zhang
7/2016-12/2017	Predicting Structure-Property Relationships in Optoelectronic Materials, NSF XSEDE, CHE140101, Computer time valued $15,237.00, PI: Levine
4/2016	GPU-Accelerated Modeling of the Non-Radiative Dynamics of Excited Nanomaterials, NVidia Professor Partnership, computer hardware valued ~$3,500, PI: Levine
10/2014-10/2015	GPU-Accelerated Modeling of Non-Radiative Recombination in Materials for Optoelectronic Applications, NSF XSEDE, CHE140101, Computer time valued $14,188.90, PI: Levine
8/2012	GPU-Accelerated Modeling of the Non-Radiative Dynamics of Excited Nanomaterials, NVidia Professor Partnership, computer hardware valued ~$2,000, PI: Levine

Postdoctoral Advisees (Current position in parenthesis if known)

2023-present	Jiří Suchan
2021-present	Arshad Mehmood
2021-2022	Alexander Teplukhin (Intel)
2020-2021	Michael P. Esch
2017-2020	Dmitry A. Fedorov (Walgreen's Data Science)

Graduate Student Advisees (Current position in parenthesis if known)

2023-present	Eric Marants
2023-present	Ari Pereira

2022-present	Ying You
2021-present	Thomas Knoll
2020-present	Caitlin Hetherington
2017-2024	Fangchun Liang, Ph.D. (Postoctoral Researcher, Cleveland Clinic)
2021-2023	Kenneth Berard, M.S. (Ph.D. Student, Rubenstein group, Brown University)
2017-2023	Andrew Durden, Ph.D. (Postdoctoral Researcher, Schlegel group, Wayne State University)
2015-2020	Michael P. Esch, Ph.D.
2022-2024	Satoshi Ohtsuka, M.S. (Ph.D. student, University of Texas)
2019-2020	Kathryn Humphries, M.S., co-adviser Prof. Jim McCusker (Ph.D. student in Ojima group at Stony Brook University)
2016-2020	Dylan T. Hardwick, M.S.
2014-2019	Wei-Tao Peng, Ph.D. (Assistant Professor, Tunghai University, Taiwan)
2014-2017	Brandon Z. Child, M.S.
2012-2017	B. Scott Fales, Ph.D. (QCWare)
2011-2016	Garrett A. Meek, Ph.D. (Abbvie)
2011-2016	Yinan Shu, Ph.D. (Postdoctoral Researcher, Truhlar Group, U. Minnesota)

Undergraduate Research Advisees (Current position or future degree earned in parenthesis)

2025-present	Shiva Sai Teja Kalva
2023-present	Zain Zaidi
Summer 2024	Ubaidullah Hassan (undergraduate student, Cooper Union)
2023-2024	Iulianna Taradachuk
Summer 2023	Peter Scully (Undergraduate Student, Tufts University)
2022-2023	Pen Chang Chang (Ph.D. student, Yale University
Summer 2022	Michael Rivera-Lazu (Ph.D. student, Tufts University)
Summer 2021	Kevin Torres (Ph.D. student, New York University)
Summer 2021	Trevor Lata
2020-2021	Gabriella Albanese
Summer 2019	Andrew LaDuca (Ph.D. student, U. Michigan)
2016-2018	Derek Metcalf (CSO, Lavo Life Sciences)
Summer 2016	Tiffany Rivera
2015-2016	David Bianchi (Ph.D. University of Illinois)
2014-2015	Benjamin Thompson
Summer 2014	Michael Esch (Ph.D. Michigan State University)
2013-2014	Monica O'Brien (Pfizer)
2013	Nick Baker
2011-2014	Oskar Ubysz (M.D., Jagiellonian University, Poland)

High School Advisees

2023	Xin Qi Liu (MIT)

Summer 2016 Fardowsa Omar

Editorial Activities

- Associate Editor, Chemical Physics Reviews, 2025-present
- Editorial Advisory Board member, Journal of Chemical Physics, 2020-2022
- Editorial Advisory Board member, Journal of Physical Chemistry, 2018-2020
- Guest editor of a special issue of the International Journal of Quantum Chemistry on Excited States of Complex Systems, published 3/2016, http://dx.doi.org/10.1002/qua.v116.10 (Co-editing with Prof. Sergey Varganov, University of Nevada at Reno)
- Reviewer for Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Journal of Chemical Physics, Chemical Physics, Physical Chemistry Chemical Physics, Chemical Physics Letters, Journal of Computational Chemistry, Journal of Chemical Information and Modeling, Advanced Materials, Nature Materials, Communications Chemistry, Nanoscale, Chemistry of Materials, Chemical Reviews, Journal of the American Chemical Society, RCS Chemical Science, Accounts of Chemical Research, Journal of Organic Chemistry, Inorganic Chemistry, Journal of Molecular Modeling, Diamond and Related Materials

Conference Organization

- As PHYS division program chair, will oversee ACS PHYS division program at the 2027 Spring and ACS Fall National Meetings.
- Organizing symposium titled “Charge Transfer and Energy Conversion at Interfaces and Defects” at the Spring 2023 National Meeting of the American Chemical Society in Indianapolis (Co-organizing with Sahar Sharifzadeh, Boston U. and Pengfei Huo, U. Rochester)
- Organized symposium titled “Modeling dynamics in dense manifolds of states” at the Spring 2019 National Meeting of the American Chemical Society in Orlando (Co-organizing with Petr Slavicek, University of Chemistry and Technology, Prague)
- Organized the 49th annual Midwest Theoretical Chemistry Conference, held in East Lansing, MI, June 1-3, 2017
- Organized symposium titled “Preparing for the Real World: Challenges Faced by Young Investigators” at the Spring 2016 National Meeting of the American Chemical Society in San Diego (Co-organizing with Sereina Riniker, ETH Zurich, and Dominika Zgid, University of Michigan)
- Served on Young Chemists Committee for the organization of the Spring 2016 National Meeting of the American Chemical Society, themed “Computers in Chemistry”
- Organized symposium titled “Modeling Excited States of Complex Systems” at the Spring 2015 Meeting of the American Chemical Society in Denver (Co-organized with Prof. Sergey Varganov, University of Nevada at Reno)

Professional Societies

- Vice Chair Elect of the PHYS division of the American Chemical Society, 2025 (will continue to serve as Vice Chair, Chair Elect, Chair, and Past Chair in 2026-2029, respectively)
- Chair of the Energy Subdivision of the American Chemical Society, 2023
- Chair Elect of the Energy Subdivision of the American Chemical Society, 2022
- Vice Chair of the Energy Subdivision of the American Chemical Society, 2021
- Treasurer of the Michigan State University section of the American Chemical Society, 2014-2020
- Chair of the Michigan State University section of the American Chemical Society, 2013
- Chair-elect of the Michigan State University section of the American Chemical Society, 2012
- American Chemical Society, COMP and PHYS division member
- American Physical Society, DAMOP member

Other Professional Activities

- Participant in NSF Workshop on Future Directions of the Cyberinfrastructure for Sustained Scientific Innovation (CSSI) Program, October 29-30, 2019, Austin, TX
- Grant Reviewer and/or Panelist for Air Force Office of Scientific Research, U.S. Department of Energy, National Science Foundation, American Chemical Society Petroleum Research Fund, Research Corporation, Natural Sciences and Engineering Research Council (Canada), European Research Council, and others

University, College, and Departmental Services

- Empire Innovation Program Computational Materials Search Committee, Spring 2025
- Physical Chemistry Search Committee, Chair, Fall 2024-Spring 2025
- Chemistry Department Graduate Admissions Committee, Fall 2021-present
- IACS Leadership Team, Fall 2020-present
- Chemistry Department Strategic Planning, Spring 2022-Spring 2024
- Chemistry Department Graduate Recruiting Committee, Fall 2020-Spring 2024
- IACS Junior Researcher Award Committee, Spring 2022, 2023
- IACS Postdoctoral Fellowship Committee, Spring 2021, 2022, 2023, 2024
- IACS Graduate Fellowship Committee, Spring 2021, 2022, 2023, 2024
- IACS New Recruit Award Committee, Spring 2023
- Materials Science and Chemical Engineering Search Committee, Fall 2022-Spring2023
- Chemistry Department Search Committee, Fall 2022-Spring 2023
- College of Arts and Sciences Data Literacy Working Group, Fall 2021
- Chair, Department of Chemistry Faculty Advisory Committee, Fall 2019-Winter 2020; Member, Fall 2011-Fall-2013, Summer 2019-Winter 2020

- Chairperson Search Committee for the Department of Chemistry, Spring 2019-Winter 2020
- Department of Chemistry Strategic Planning Committee, Spring 2019-Summer 2019
- Soft Electronic Materials Search Committee for the Department of Chemical Engineering and Materials Science, Fall 2018-Summer 2019
- Graduate Advising, Fall 2013-Spring 2015, Fall 2016, Fall 2019
- Graduate Admissions Committee, Fall 2012-Spring 2014, Fall 2015-Spring 2016, Fall 2018-Spring 2019
- Department of Chemistry Undergraduate Affairs Committee, Fall 2018-Fall 2019
- Organizer for Physical Chemistry Seminar Series, Fall 2012-present (co-organized by Prof. Heedeok Hong since Fall 2013)
- Guidance Committee for Tom Carter, Fall 2011-present
- Institute for Cyber-Enabled Research Scientific Advisory Board, Fall 2013-present
- Organizer for Complex Materials Seminar Series, Spring 2015-Spring 2016 and Fall 2018 (co-organized by Prof. Rémi Beaulac in Spring 2015, Prof. Phillip Duxbury in Fall 2015 and Spring 2016, and Prof. Rebecca Anthony in Fall 2018)
- Planning Committee, Spring 2016, Summer 2017
- Computational Chemistry Search Committee for the Department of Chemistry, Fall 2014-Spring 2015
- College of Natural Sciences committee to write a proposal for the Department of Computational Mathematics, Science, and Engineering, Spring 2014-Sping 2015
- Organizing Committee of the Midwestern Symposium on Undergraduate Research, 2011, 2012, and 2014

Classes Taught

- Spring semester 2025 – CHE 525/PHY 567 – Theoretical Chemistry/Theoretical Chemical Physics
- Fall semester 2024 – CHE 351/521 – Quantum Chemistry I
- Spring semester 2024 – CHE 525/PHY 567 – Theoretical Chemistry/Theoretical Chemical Physics
- Fall semester 2023 – CHE 351/521 – Quantum Chemistry I
- Spring semester 2023 – CHE 525/PHY 567 – Theoretical Chemistry/Theoretical Chemical Physics
- Fall semester 2022 – CHE 351/521 – Quantum Chemistry I
- Spring semester 2022 – CHE 525/PHY 567 – Theoretical Chemistry/Theoretical Chemical Physics
- Spring semester 2021 – CHE 525 – Theoretical Chemistry
- Spring semester 2020 – CEM 384 – Introduction to Physical Chemistry II
- Spring semester 2019 – CEM 384 – Introduction to Physical Chemistry II
- Fall semester 2018 – CEM 883 – Computational Quantum Chemistry
- Fall semester 2018 – CEM 998 – Physical Chemistry Seminar
- Spring semester 2018 – CEM 998 – Physical Chemistry Seminar

- Spring semester 2017 – CEM 182H – Honors Freshman Chemistry
- Spring semester 2017 – CEM 998 – Physical Chemistry Seminar
- Fall semester 2017 – CEM 883 – Computational Quantum Chemistry
- Spring semester 2016 – CEM 182H – Honors Freshman Chemistry
- Spring semester 2016 – CEM 998 – Physical Chemistry Seminar
- Spring semester 2015 – CEM 182H – Honors Freshman Chemistry
- Spring semester 2015 – CEM 998 – Physical Chemistry Seminar
- Spring semester 2014 – CEM 182H – Honors Freshman Chemistry
- Fall semester 2013 – CEM 883 – Computational Quantum Chemistry
- Fall semester 2013 – CEM 998 – Physical Chemistry Seminar
- Spring semester 2013 – CEM 182H – Honors Freshman Chemistry
- Spring semester 2013 – CEM 998 – Physical Chemistry Seminar
- Fall semester 2012 – CEM 998 – Physical Chemistry Seminar
- Fall semester 2011 – CEM 883 – Computational Quantum Chemistry

Publication Statistics (from Google Scholar, 3/7/2025)

Total citations: **7582**
Total citations in 2024: **648**
h-index: **38**

Publications

93. Bottom-up Carbon Dots: Purification, Single-Particle Dynamics, and Electronic Structure, Z. Bian, E. Gomez, M. Gruebele, B. G. Levine, S. Link, A. Mehmood, and S. Nie, Chem. Sci., **16**, 4195 (2025)

92. Long-Lived Electronic Coherences from First Principles, J. Suchan and B. G. Levine, submitted (2025) https://doi.org/10.48550/arXiv.2502.04494

91. Factors Governing H3+ Formation from Methyl Halogens and Pseudohalogens, J. Stamm, S. S. Priyadarsini, S. Sandhu, A. Chakraborty, J. Shen, S. Kwon, J. Sandhu, C. Wicka, A. Mehmood, B. G. Levine, P. Piecuch, and M. Dantus, Nat. Commun. **16**, 410 (2025)

90. Efficient and Scalable Wave Function Compression Using Corner Hierarchical Matrices, K. O. Berard, H. Gao, A. Teplukhin, X. Jiao, and B. G. Levine, J. Chem. Phys. **161**, 204106 (2024)

89. Simulating Passage through a Cascade of Conical Intersections with Collapse-to-a-Block Molecular Dynamics, F. Liang and B. G. Levine, Mol. Phys. e2428815 (2024) (Special Issue in honor of Piotr Piecuch)

88. The Role of the Plasmon in Interfacial Charge Transfer, B. Ostovar, S. A. Lee, A. Mehmood, K. Farrell, E. K. Searles, B. Bourgeois, W.-Y. Chiang, A. Misiura, N. Gross, A. Al-

Zubeidi, J. A. Dionne, C. F. Landes, M. Zanni, B. G. Levine, and S. Link, Sci. Adv. **10**, eadp3353 (2024)

87. Ab Initio Multiple Spawning Nonadiabatic Dynamics with Different CASPT2 Flavors: A Fully Open-Source PySpawn/OpenMolcas Interface, L. Ibele, A. Mehmood, B. G. Levine, and D. Avagliano, J. Chem. Theory Comput. **20**, 8140 (2024)

86. Coherence Mapping to Identify the Intermediates of Multi-Channel Dissociative Ionization, J. Stamm, S. Kwon, S. Sandhu, J. Sandhu, B. G. Levine, and M. Dantus, Comm. Chem. **7**, 103 (2024)

85. Resonance Effects from Substituents on L-Type Ligands Mediate Synthetic Control of Gold Nanocluster Frontier Orbital Energies, H. Morales Hernández, S. Ohtsuka, A. Mehmood, J. Bordenca, W. Wen, B. G. Levine, and C. J. Johnson, J. Phys. Chem. Lett. **15**, 10244 (2024)

84. Simulating Ultrafast Transient Absorption Spectra from First Principles using a Time-Dependent Configuration Interaction Probe, A. Mehmood, M. C. Silfies, A. S. Durden, T. K. Allison, and B. G. Levine, J. Chem. Phys. **161**, 044107 (2024)

83. IR Spectroscopy of Carboxylate-Passivated Semiconducting Nanocrystals: Simulation and Experiment, J. K. Sowa, D. M. Cadena, A. Mehmood, B. G. Levine, S. T. Roberts, and P. J. Rossky, J. Phys. Chem. C., J. Phys. Chem. C, **128**, 8724 (2024)

82. Prediction Challenge: First Principles Simulation of the Ultrafast Electron Diffraction Spectrum of Cyclobutanone, J. Suchan, F. Liang, A. S. Durden, and B. G. Levine, J. Chem. Phys., **160**, 134310 (2024)

81. Origin of Vibronic Coherences During Carrier Cooling in Colloidal Quantum Dots, C. V. Hetherington, N. Mohan T. M., R. W. Tilluck, W. F. Beck, and B. G. Levine, J. Phys. Chem. Lett. **14**, 11651 (2023)

80. Properties of Carbon Dots versus Small Molecules from “Bottom-up” Synthesis, Z. Bian, A. Wallum, A. Mehmood, E. Gomez, Z. Wang, S. Pandit, S. Nie, S. Link, B. G. Levine, and M. Gruebele, ACS Nano, **17**, 22788 (2023)

79. What is the Mechanism of H3+ Formation from Cyclopropane?, S. Kwon, S. Sandhu, M. Shaik, J. Stamm, J. Sandhu, R. Das, C. V. Hetherington, B. G. Levine, M. Dantus, J. Phys. Chem. A, **127**, 8633 (2023)

78. The Surprising Dynamics of the McLafferty Rearrangement, J. Stamm, S. Kwon, S. Sandhu, M. Shaik, R. Das, J. Sandhu, B. Curenton, C. Wicka, B. G. Levine, L. Sun, M. Dantus, J. Phys. Chem. Lett., **14**, 10088 (2023)

77. Ultrafast Internal Conversion and Photochromism in Gas-Phase Salicylideneaniline, M. C. Silfies, A. Mehmood, G. Kowzan, E. G. Hohenstein, B. G. Levine, T. K. Allison, J. Chem. Phys., **159**, 104304 (2023)

76. Human Serum Albumin Dimerization Enhances the S2 Emission of Bound Cyanine IR806, J. Lahiri, S. Sandhu, B. G. Levine, and M. Dantus, J. Phys. Chem. Lett., **13**, 1825 (2022)

75. Floquet Time-Dependent Configuration Interaction for Modeling Ultrafast Electron Dynamics, A. S. Durden and B. G. Levine, J. Chem. Theory Comput., **18**, 795 (2022)

74. Consensus Statement: Standardized Reporting of Power-Producing Luminescent Solar Concentrator Performance, C. Yang, et al. Joule, **6**, 8 (2022)

73. Linear and Nonlinear Optical Processes Controlling S2 and S1 Dual Fluorescence in Cyanine Dyes, M. Laboe, J. Lahiri, N. Mohan T. M., F. Liang, B. G. Levine, W. F. Beck, and M. Dantus, J. Phys. Chem. A, **125**, 9770 (2021) (Invited Article in 125th Anniversary Virtual Special Issue)

72. An Accurate, Non-empirical Method for Incorporating Decoherence into Ehrenfest Dynamics, M. P. Esch and B. G. Levine J. Chem. Phys. **155**, 214101 (2021)

71. Vibronic Excitons and Conical Intersections in Semiconductor Quantum Dots, R. W. Tilluck, N. Mohan T. M., C. V. Hetherington, C. H. Leslie, S. Sil, J. Frazier, M. Zhang, B. G. Levine, P. G. Van Patten, and W. F. Beck, J. Phys. Chem. Lett. **12**, 9677 (2021)

70. CAS without SCF—Why to Use CASCI and Where to Get the Orbitals, B. G. Levine, A. S. Durden, M. P. Esch, F. Liang, and Y. Shu, J. Chem. Phys. **154**, 090902 (2021) Perspective Article

69. General Strategy for Tuning the Stokes Shifts of Near Infrared Cyanine Dyes, J. Zhang, M. Moemeni, C. Yang, F. Liang, W.-T. Peng, B. G. Levine, R. Lunt, and B. Borhan J. Mater. Chem. C, J. Mater. Chem. C, **8**, 16769 (2020) (HOT Paper)

68. Decoherence-Corrected Ehrenfest Molecular Dynamics on Many Electronic States, M. P. Esch and B. G. Levine, J. Chem. Phys. **153**, 114104 (2020)

67. PySpawn: Software for Nonadiabatic Quantum Molecular Dynamics, D. A. Fedorov, S. Seritan, B. S. Fales, T. J. Martínez, and B. G. Levine, J. Chem. Theory Comput., **16**, 5485 (2020)

66. State-Pairwise Decoherence Times for Nonadiabatic Dynamics on More Than Two Electronic States, M. P. Esch and B. G. Levine, J. Chem. Phys. **152**, 234105 (2020) (JCP Editors' Pick)

65. Electronic and Structural Comparisons between Iron(II/III) and Ruthenium(II/III) Imide Analogs, K. E. Aldrich, B. S. Fales, A. K. Singh, R. J. Staples, B. G. Levine, J. McCracken, M. R. Smith III, and A. L. Odom, Inorg. Chem., **58**, 11699 (2019)

64. Nonadiabatic Quantum Molecular Dynamics in Dense Manifolds of Electronic States, D. A. Fedorov and B. G. Levine, J. Phys. Chem. Lett., **10**, 4542 (2019)

63. Ab Initio Molecular Dynamics Study of the Interaction Between Defects During Nonradiative Recombination, W.-T. Peng and B. G. Levine, J. Phys. Chem. C., **123**, 16588 (2019)

62. Locality of Conical Intersections in Semiconductor Nanomaterials, B. G. Levine, W.-T. Peng, and M. P. Esch, Phys. Chem. Chem. Phys., **21**, 10870 (2019) (PCCP HOT Article for 2019)

61. A Conical Intersection Perspective on the Low Nonradiative Recombination Rate in Lead Halide Perovskites, M. P. Esch, Y. Shu, and B. G. Levine J. Phys. Chem. A, **123**, 2661 (2019)

60. A Discontinuous Basis Enables Numerically Exact Solution of the Schrödinger Equation around Conical Intersections in the Adiabatic Representation, D. A. Fedorov and B. G. Levine, J. Chem. Phys., **150**, 054102 (2019)

59. Conical Intersections at the Nanoscale: Molecular Ideas for Materials, B. G. Levine, M. P. Esch, B. S. Fales, D. T. Hardwick, W.-T. Peng, and Y. Shu, Ann. Rev. Phys. Chem., **70**, 21 (2019)

58. Substituent Effects on H3+ Formation via H2 Roaming Mechanisms from Organic Molecules under Strong-Field Photodissociation, N. Ekanayake, M. Nairat, N. P. Weingartz, M. J. Michie, B. G. Levine, and M. Dantus, J. Chem. Phys., **149**, 244310 (2018) (Featured Article)

57. H2 Roaming Chemistry and the Formation of H3+ from Organic Molecules in Strong Laser Fields, N. Ekanayake, T. Severt, M. Nairat, N. P. Weingartz, B. M. Farris, B. Kaderiya, P. Feizollah, B. Jochim, F. Ziaee, K. Borne, K. Raju P., K. D. Carnes, D. Rolles, A. Rudenko, B. G. Levine, J. E. Jackson, I. Ben-Itzhak, and M. Dantus, Nat. Commun., **9**, 5186 (2018)

56. Impact of Stokes Shift on the Performance of Near-Infrared Harvesting Transparent Luminescent Solar Concentrators, C. Yang, J. Zhang, W.-T. Peng, W. Sheng, D. Liu, P. S. Kuttipillai, M. Young, M. R. Donahue, B. G. Levine, B. Borhan, and R. R. Lunt, Sci. Rep., **8**, 16359 (2018)

55. Large Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction, B. S. Fales, S. Seritan, N. F. Settje, B. G. Levine, H. Koch, and T. J. Martínez, J. Chem. Theory Comput., **14**, 4139 (2018)

54. Simulating Electron Dynamics of Complex Molecules with Time-Dependent Complete Active Space Configuration Interaction, W.-T. Peng, B. S. Fales, and B. G. Levine, J. Chem. Theory Comput., **14**, 4129 (2018)

53. Dynamics of Recombination via Conical Intersection in a Semiconductor Nanocrystal, W.-T. Peng, B. S. Fales, Y. Shu, and B. G. Levine, Chem. Sci., **9**, 681 (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. Understanding Non-Radiative Recombination through Defect-Induced Conical Intersections, Y. Shu, B. S. Fales, W.-T. Peng, and B. G. Levine, J. Phys. Chem. Lett., **8**, 4091 (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. Mechanisms and time-resolved dynamics for trihydrogen cation (H_3^+) formation from organic molecules in strong laser fields, N. Ekanayake, M. Nairat, B. Kaderiya, P. Feizollah, B. Jochim, T. Severt, B. Berry, K. R. Pandiri, K. D. Carnes, S. Pathak, D. Rolles, A. Rudenko, I. Ben-Itzhak, C. A. Mancuso, B. S. Fales, J. E. Jackson, B. G. Levine, and M. Dantus, Sci. Rep., **7**, 4703 (2017)

48. Time-Resolved Signatures Across the Intramolecular Response in Substituted Cyanine Dyes, M. Nairat, M. Webb, M. P. Esch, V. V. Lozovoy, B. G. Levine, and M. Dantus, Phys. Chem. Chem. Phys., **19**, 14085 (2017)

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

46. The Best of Both Reps: Diabatized Gaussians on Adiabatic Surfaces, G. A. Meek and B. G. Levine, J. Chem. Phys., **145**, 184103 (2016)

45. First Principles Study of Non-Radiative Recombination in Silicon Nanocrystals: The Role of Surface Silanol, Y. Shu and B. G. Levine, J. Phys. Chem. C, **120**, 23246 (2016)

44. Wave Function Continuity and the Diagonal Born-Oppenheimer Correction at Conical Intersections, G. A. Meek and B. G. Levine, J. Chem. Phys., **144**, 184109 (2016)

43. Special Issue on Excited States of Complex Materials, B. G. Levine and S. A. Varganov, Int. J. Quant. Chem., **116**, 737 (2016)

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39. Defect-Induced Conical Intersections Promote Nonradiative Recombination, Y. Shu, B. S. Fales, and B. G. Levine, Nano Lett., **15**, 6247 (2015)

38. Accurate and efficient evaluation of transition probabilities at unavoided crossings in ab initio multiple spawning, G. A. Meek and B. G. Levine, Chem. Phys., **460**, 117 (2015) (Special Issue on the Jahn-Teller Effect)

37. Simulated evolution of fluorophores for light emitting diodes, Y. Shu and B. G. Levine, J. Chem. Phys., **142**, 104104 (2015)

36. 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)

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32. Steric and electrostatic effects on photoisomerization dynamics using QM/MM ab initio multiple spawning. A. M. Virshup, B. G. Levine, and T. J. Martinez, Theor. Chem. Acc., **133**, 1506 (2014)

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30. Do excited silicon-oxygen double bonds emit light? Y. Shu, B. G. Levine, J. Phys. Chem. C, **118**, 7669 (2014)

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26. Determining the lowest-energy isomer of Au_8: 2D, or not 2D. J. A. Hansen, P. Piecuch, B. G. Levine, J. Chem. Phys., **139**, 091101 (2013)

25. Non-radiative recombination via conical intersection at a semiconductor defect. Y. Shu, B. G. Levine, J. Chem. Phys., **139**, 081102 (2013)

24. Reducing the propensity for unphysical wavefunction symmetry breaking in multireference calculations of the excited states of semiconductor clusters. Y. Shu, B. G. Levine, J. Chem. Phys., **139**, 074102 (2013)

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* These authors contributed equally to this work.

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* These authors contributed equally to this work.

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* These authors contributed equally to this work.

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* These authors contributed equally to this work.

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* These authors contributed equally to this work.

17. Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus, R. Acharya*, V. Carnevale*, G. Fiorin*, B. G. Levine*, A. L. Polishchuk*, V. Balannik, I. Samish, R. A. Lamb, L. H. Pinto, W. F. DeGrado, M. L. Klein, Proc. Natl. Acad. Sci. U.S.A., **107**, 15075 (2010)
* These authors contributed equally to this work.

16. Functional studies and modeling of an extensive set of mutants of pore-lining residues of the M2 ion channel of influenza A virus. V. Balannik, V. Carnevale, G. Fiorin, B. G. Levine, R. A. Lamb, M. L. Klein, W. F. DeGrado, and L. H. Pinto, Biochemistry, **49**, 696 (2010)

15. Ab Initio Multiple Spawning Dynamics using Multi-State Second-Order Perturbation Theory, H. Tao, B. G. Levine, and T. J. Martínez, J. Phys. Chem. A, **113**, 13656 (2009)

14. Ab Initio Multiple Spawning Dynamics of Excited Butadiene: The Role of Charge Transfer, B. G. Levine and T. J. Martínez, J. Phys. Chem. A, **113**, 12815 (2009)

13. On the Extent and Connectivity of Conical Intersection Seams and the Effects of Three-State Intersections, J. D. Coe, M. T. Ong, B. G. Levine, and T. J. Martínez, J. Phys. Chem. B, **112**, 12559 (2008)

12. Optimizing Conical Intersections Without Derivative Coupling Vectors: Application to Multi-State Multireference Second Order Perturbation Theory (CASPT2), B. G. Levine, J. D. Coe, and T. J. Martínez, J. Phys. Chem. B, **112**, 405 (2008)

11. Implementation of Ab Initio Multiple Spawning in the MolPro Quantum Chemistry Package, B. G. Levine, J. D. Coe, A. Virshup, and T. J. Martínez, Chem. Phys., **347**, 3 (2008)

10. Ab Initio Molecular Dynamics and Time-Resolved Photoelectron Spectroscopy of Electronically Excited Uracil and Thymine, H. R. Hudock, B. G. Levine, A. L. Thompson, H. Satzger, D. Townsend, N. Gador, S. Ullrich, A. Stolow, and T. J. Martínez, J. Phys. Chem. A, **111**, 8500 (2007)

9. Ab Initio Molecular Dynamics of Excited State Intramolecular Proton Transfer Using Multireference Perturbation Theory, J. D. Coe, B. G. Levine, and T. J. Martínez, J. Phys. Chem. A, **111**, 11302 (2007)

8. Isomerization through Conical Intersections, B. G. Levine and T. J. Martínez, Ann. Rev. Phys. Chem., **58**, 613 (2007)

7. First Principles Dynamics of Photoexcited DNA and RNA Bases, H. R. Hudock, B. G. Levine, A. L. Thompson, and T. J. Martínez, AIP Conf. Proc., **963**, 219 (2007)

6. Conical Intersections and Double Excitations in Time-Dependent Density Functional Theory, B. G. Levine, C. Ko, J. Quenneville, and T. J. Martínez, Mol. Phys., **104**, 1053 (2006)

5. Photochemistry from First Principles and Direct Dynamics, A. Toniolo, B. Levine, A. Thompson, J. Quenneville, M. Ben-Nun, J. Owens, S. Olsen, L. Manohar, and T. J. Martínez, Computational Methods in Photochemistry, ed. A. Kutateladze, 2005, pp. 167-234

4. First Principles Ab Initio Multiple Spawning Dynamics of Electronically Excited trans-1,3-Butadiene with Wavefunction and Density Functional Theory, B. Levine and T. J. Martínez, in Quantum Dynamics and Conical Intersections, Ed. G. A. Worth and S. C. Allthorpe, Daresbury, CCP6 (2004)

3. Ab Initio Multiple Spawning Dynamics of the Photoactive Yellow Protein Chromophore, C. Ko, B. Levine, L. Manohar, S. Olsen, and T. J. Martínez, J. Am. Chem. Soc., **125**, 12710 (2003)

2. Quantum Energy Flow and *trans*-Stilbene Photoisomerization: A Textbook Example of a non-RRKM Reaction? D. M. Leitner, B. Levine, J. Quenneville, T. J. Martínez, and P. G. Wolynes, J. Phys. Chem., **107**, 10706 (2003)

1. Mechanism and Dynamics of Azobenzene Photoisomerization, T. Schultz, J. Quenneville, B. Levine, A. Toniolo, T. J. Martínez, S. Lochbrunner, M. Schmitt, J. P. Shaffer, M. Z. Zgierski, and A. Stolow, J. Am. Chem. Soc., **125**, 8098 (2003)

Patents

Lunt, Richard R., Babak Borhan, Benjamin G. Levine, Wei Sheng, Jun Zhang, and Chenchen Yang. Near-Infrared Harvesting Transparent Luminescent Solar Concentrators with Engineered Stokes Shift. U.S. Patent US20210230427A1, filed May 9, 2018.

Popular Publications

Půjčte vědcům Playstation... a už vám ji nevrátí (translated: Loan a Scientist a Playstation... and he may never return it), B. Levine and P. Slavicek, published in ABC (Czech magazine for young scientists)

Invited Talks (since August 2011)

89. Chemistry Department Seminar, Texas Tech University, Lubbock, TX, Nov 2024 – "First Principles Simulation of Coherent Dynamics on Many Electronic States"

88. Invited Talk, Congress of the International Society for Theoretical Chemical Physics, Qingdao, China, Oct 2024 – “Ultrafast Dynamics on Many Electronic States”

87. Invited Talk, American Physical Society Division of Atomic, Molecular, and Optical Physics (DAMOP) Meeting, Fort Worth, TX, Jun 2024 – “Ab Initio Molecular Dynamics on Many Electronic States”

86. Theoretical Chemistry Seminar, University of Chemistry and Technology, Prague, Czech Republic, Jun 2024 – “Ab Initio Molecular Dynamics on Many Electronic States”

85. IMPRS for Quantum Dynamics and Control Seminar, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, May 2024 – “Connecting Ultrafast Spectra to Ultrafast Dynamics”

84. Chemistry Department Seminar, Oregon State University, Corvallis, OR, Apr 2024 – “Connecting Ultrafast Spectra to Ultrafast Dynamics”

83. CUNY Initiative for Theoretical Sciences Workshop on First Principles Quantum Dynamics Calculations of and on Many-Electron States, New York, NY, Apr 2024 – “Ab Initio Molecular Dynamics on Many Electronic States”

82. Chemistry Department Seminar, Queens College (CUNY), Queens, NY, Apr 2024 – “Connecting Ultrafast Spectra to Ultrafast Dynamics”

81. American Chemical Society National Meeting, New Orleans, LA, Mar 2024 – “Theory of Conical Intersections as a Tool for Nanoscience”

80. American Chemical Society National Meeting, New Orleans, LA, Mar 2024 – “Ab Initio Molecular Dynamics on Many Electronic States”

79. Boston Area Theoretical Chemistry Seminar, Cambridge, MA, Dec 2023 – “Ab Initio Molecular Dynamics on Many Electronic States”

78. Physics Department Seminar, Rutgers University-Newark, Newark, NJ, Nov 2023 – “Ab Initio Molecular Dynamics on Many Electronic States”

77. Telluride Workshop on Nonadiabatic Dynamics, Telluride, CO, Oct 2023 – “Ab Initio Molecular Dynamics on Many Electronic States”

76. Wintergreen Physical Chemistry Conference, Wintergreen, VA, Sept 2023 – “Theory of Conical Intersections as a Tool for Nanoscience”

75. Dynamics of Molecular Collisions, Snowbird, UT, July 2023 – “Nonadiatbiatic Dynamics – Session Introduction”

74. Chemistry Department Seminar, University of California at San Diego, CA, May 2023 – "Connecting Ultrafast Spectra to Ultrafast Dynamics"

73. Chemistry Department Seminar, Wesleyan University, CT, Feb 2023 – "Connecting Ultrafast Spectra to Ultrafast Dynamics"

72. Keynote Lecture at Stony Brook University Chemistry Research Day, Stony Brook, NY, Oct 2022 – "Connecting Ultrafast Spectra to Ultrafast Dynamics"

71. CHAMPS Workshop on Roaming, East Lansing, MI, Oct 2022 – "Roaming Mechanism For H_3^+ Formation from Methanol and Ethanol"

70. Pennsylvania State University Theoretical Chemistry Seminar, State College, PA, Sept 2022 – "Connecting Ultrafast Spectra to Ultrafast Dynamics"

69. TeraChem Developers Workshop, Lake Tahoe, CA, July 2022 – "Levine Group Update"

68. Gordon Research Conference on Molecular Interactions and Dynamics, Stonehill College, MA, July 2022 – "Connecting Theory to Experiment: First Principles Simulation of Transient Absorption Spectra"

67. Mid-Atlantic Regional Meeting of the American Chemical Society, Trenton, NJ, June 2022 – "Toward Accurate Nonadiabatic Molecular Dynamics on Many-Electronic States"

66. New York University-Shanghai/East China Normal University Center for Theoretical Chemistry Seminar, Online, Apr 2022 – "Toward Accurate Ab Initio Molecular Dynamics on Many Electronic States"

65. Centre Européen de Calcul Atomique et Moléculaire (CECAM) Workshop on Exciton Dynamics in Functional Materials, Online, Dec 2021 – "Nonradiative Recombination Through Conical Intersections"

64. Johns Hopkins University Chemistry Department Seminar, Baltimore, MD, Nov 2021 – "Nonradiative Recombination through Conical Intersections"

63. National Meeting of the American Chemical Society, online, Aug 2021 – "Nonradiative Recombination Through Conical Intersections"

62. DOE Computational and Theoretical Chemistry Research PI Meeting (CTC), online, Aug 2021 – "Nonadiabatic Molecular Dynamics on Many Electronic States"

61. Telluride Science Research Center Workshop on Nonequilibrium Phenomena, Nonadiabatic Dynamics, and Spectroscopy, online, Jul 2021 – “Nonadiabatic Molecular Dynamics on Many Electronic States”

60. World of Physics, Stony Brook University (general audience talk), online, Apr 2021 – “Better Living Through Quantum Mechanics and Computers (…and Chemistry)”

59. Stony Brook Institute for Advanced Computational Science Research Day, online, Apr 2021 – “Molecular Dynamics on Many Electronic States”

58. Brookhaven National Lab, Center for Functional Nanomaterials, Theory Seminar, online, Feb 2021 – “Conical Intersections in Semiconductor Nanocrystals—How is Electronic Energy Converted to Heat?”

57. Stony Brook Chemistry Research Day, online, Feb 2021 – “Defects as Molecules - Using Chemical Theory to Understand Semiconductor Photophysics”

56. Rowan University Chemistry Department Seminar, online, Nov 2020 – “Semiconductor Nanomaterials - How is Electronic Energy Lost as Heat?”

55. Stony Brook University Condensed Matter Physics Seminar, online, Oct 2020 – “Conical Intersections in Semiconductor Nanocrystals—How is Electronic Energy Converted to Heat?”

54. TeraChem Developers’ Workshop, online, Sept 2020 – “Levine Group Update”

53. Retirement Symposium for NSF Program Officer Evi Goldfield, online, Sept 2020 – “The Best of Both Reps – Diabatized Gaussians on Adiabatic Surfaces”

52. Low-Scaling and Unconventional Structure Techniques Conference (LUEST), online, June 2020 – “Toward Ab Initio Molecular Dynamics on Many Electronic States”

51. Sanibel Symposium, St. Simons Island, GA, Feb 2020 – “Toward Ab Initio Molecular Dynamics on Many Electronic States”

50. Seminar at Dept. of Chemistry and Institute for Advanced Computational Science, Stony Brook University, Stony Brook, NY, Nov. 2019 – “How is Electronic Energy Converted to Heat in Semiconductor Nanocrystals”

49. Seminar at Dept. of Chemistry, Emory University, Atlanta, GA, Oct. 2019 – “Nonradiative Processes in Semiconductor Nanocrystals”

48. Seminar at Dept. of Chemistry, Ohio State University, Columbus, OH, Oct. 2019 – “Nonradiative Processes in Semiconductor Nanocrystals”

47. Current Trends in Theoretical Chemistry, Krakow, Poland, Sept. 2019 – “Toward Ab Initio Molecular Dynamics on Many Electronic States”

46. DOE Computational and Theoretical Chemistry Research PI Meeting (CTC), Gaithersburg, MD, May 2019 – “Toward Ab Initio Quantum Molecular Dynamics in Dense Manifolds of Electronic States”

45. AFOSR Molecular Dynamics Program Review, Washington, DC, May 2019 – “Toward Ab Initio Molecular Dynamics on Many Electronic States”

44. Seminar, Quantum Theory Project, University of Florida, Gainesville, FL, Apr. 2019 – “Painless modeling of nonadiabatic dynamics near conical intersections and in dense manifolds of states”

43. National Meeting of the American Chemical Society, Orlando, FL, Apr. 2019 – “Modeling dynamics of strongly correlated systems with graphics processing unit–accelerated time-dependent multireference methods”

42. National Meeting of the American Chemical Society, Boston, MA, Aug. 2018 – “Defect-induced conical intersections in semiconductor nanocrystals”

41. Seminar at Dept. of Chemistry, University of Michigan at Flint, Flint, MI, April 2018 – “Conical Intersections and Non-Radiative Recombination in Nanomaterials”

40. JPCA-PHYS Lectureship at National Meeting of the American Chemical Society, Washington, DC, Aug. 2017 – “Conical Intersections and Non-Radiative Recombination in Nanomaterials”

39. American Conference of Theoretical Chemistry, Boston, MA, July 2017 – “Conical Intersections and Non-Radiative Recombination in Nanomaterials”

38. Dynamics of Molecular Collision 2017, Tahoe City, CA, July, 2017 – “Painless Modeling of Dynamics Near Conical Intersections”

37. National Meeting of the American Chemical Society, San Francisco, CA, April 2017 – “Conical Intersections and Non-Radiative Recombination in Nanomaterials”

36. National Meeting of the American Chemical Society, San Francisco, CA, April 2017 – “Painless Modeling of Dynamics Near Conical Intersections”

35. Seminar at Dept. of Chemistry, University of Nevada, Reno, NV, November 2016 – “Conical Intersections and Non-Radiative Recombination in Nanomaterials”

34. Seminar at Dept. of Chemistry, Michigan State University, East Lansing, MI, November, 2016 – “Conical Intersections and Non-Radiative Recombination in Nanomaterials”

33. National Meeting of the American Chemical Society, Philadelphia, PA, August 2016 – “First Principle Evolution of Emitters for Organic Light Emitting Diodes”

32. Ninth Congress of the International Society for Theoretical Chemical Physics, Grand Forks, ND, July 2016 – “Multireference Quantum Chemistry and Conical Intersections at the Nanoscale”

31. Midwest Theoretical Chemistry Conference, Pittsburgh, PA, June 2016 – “Conical Intersections and Non-Radiative Recombination in Nanomaterials”

30. Seminar at Dept. of Chemistry, University of Minnesota, Minneapolis, MN, May 2016 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

29. National Meeting of the Materials Research Society, Symposium on Silicon Nanostructure—Doping, Interface Effects and Sensing, Phoenix, AZ, March 2016 – “Defect-Induced Conical Intersections Facilitate Non-Radiative Recombination in Silicon Nanocrystals”

28. Seminar at Dept. of Chemistry, Washington State University, Pullman, WA, February 2016 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

27. Seminar at Dept. of Chemistry, University of Washington, Seattle, WA, February 2016 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

26. Seminar at Dept. of Chemistry, University of Toronto, Toronto, Ontario, Canada, January 2016 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

25. Pacifichem, Symposium on Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics, Honolulu, HI, December 2015 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

24. Pacifichem, Symposium on Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities, Honolulu, HI, December 2015 – “Efficient and Size-Intensive Multireference Description of the Electronic Excited States of Molecules and Nanomaterials”

23. Seminar at Dept. of Chemistry, Northwestern University, Evanston, IL, December 2015 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

22. Seminar at Dept. of Chemistry, Bowling Green State University, Bowling Green, OH, December 2015 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

21. Seminar at Center for Research Excellence in Complex Materials, Michigan State University, East Lansing, MI, October 2015 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

20. Seminar at Dept. of Chemistry, Oakland University, Auburn Hills, MI, October 2015 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

19. Seminar at Dept. of Chemistry, Stanford University, Stanford, CA, October 2015 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

18. Seminar at Dept. of Chemistry, University of California—Merced, Merced, CA, October 2015 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

17. Seminar at Dept. of Chemistry, Wayne State University, Detroit, MI, September 2015 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

16. Penn Conference on Theoretical Chemistry, Philadelphia, PA, July 2015 – "Modeling Surface Crossings at the Nanoscale"

15. Telluride Science Research Center workshop on Quantum Effects in the Condensed Phase, Telluride, CO, July 2015 – "Modeling Surface Crossings at the Nanoscale"

14. Telluride Science Research Center workshop on Excited States, Electronic Structure and Dynamics, Telluride, CO, July 2015 – "Modeling Surface Crossings at the Nanoscale"

13. Joint Great Lakes/Central Regional Meeting of the ACS symposium on Nanophotonics for Energy and Catalysis, Grand Rapids, MI, May 2015 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

12. Seminar at Dept. of Chemistry, University of Michigan, Ann Arbor, MI, February 2015 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

11. Seminar at Dept. of Chemistry, Purdue University, West Lafayette, IN, December 2014 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

10. Seminar at Dept. of Chemistry, Lehigh University, Bethlehem, PA, September 2014 – "Semiconductor Photochemistry - How is Electronic Energy Lost as Heat?"

9. Seminar at Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM, September 2014 – "Conical Intersections and Non-Radiative Recombination at Semiconductor Defects"

8. MCIAM Workshop on Multiscale Modeling and Computation of Nano-Optics, East Lansing, MI, August 2014 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

7. Telluride Science Center workshop on Excited State and Time Dependent Electronic Structure, Telluride, CO, July 2014 – “Conical Intersections and Non-Radiative Recombination at Semiconductor Defects”

6. Seminar at Dept. of Chemistry, Notre Dame, South Bend, IN, February 2014 – “Understanding Semiconductor Nanoparticles by Modeling ‘Picoparticles’”

5. Seminar at Dept. of Chemistry, Kalamazoo College, Kalamazoo, MI, November 2013 – “Understanding Semiconductor Nanoparticles by Modeling ‘Picoparticles’”

4. Seminar at Dept. of Chemistry, Western Michigan University, Kalamazoo, MI, September 2013 – “A Multireference Approach to Semiconductor Photochemistry”

3. Telluride Science Center workshop on Advances in Photoreactions, Telluride, CO, June 2013 – “A Multireference Approach to Modeling Semiconductor Photodynamics”

2. Midwestern Symposium on Undergraduate Research, East Lansing, MI, October 2012 – “Applying Computation to Understand Non-Radiative Decay in Oxygen-Containing Silicon Clusters”

1. Michigan State University Institute for Cyber-Enabled Research, East Lansing, MI, October 2011 – "What Can We Learn from Implementing Radial Distribution Function Histogramming on Several Generations of Graphics Processing Units?"

Contributed Presentations at Meetings (since August 2011; presenting speaker underlined)

Poster – C.V. Hetherington, B. G. Levine, “Shining Light on Quantum Dots”, BRIDGES: A Cross-Departmental Graduate Student Conference, Stony Brook University, Stony Brook, NY, January 2025

Talk – J. Suchan, E. Muchová, P. Slavíček, B. G. Levine, "Attosecond Processes in Aqueous Ions via Time-Dependent Quantum Chemistry" Theory around XFELs, Marseille, France, Nov 2024

Poster – Y. You, A. Mehmood, B. G. Levine, "Ultrafast Excited State Dynamics of an Octahedral Chromium(III) Coordination Complex", Chemistry Research Day, Stony Brook, NY, Oct. 2024

Poster – T. Knoll, B. G. Levine, "Advancing the Simulation of Electron Dynamics with Graphic Processing Units (GPUs) and Linear-Response Time-Dependent Density Functional Theory (LR-TDDFT)," Chemistry Research Day, Stony Brook, NY, October 2024

Poster – C.V. Hetherington, B. G. Levine, “A Conical Intersection Approach to Shining Light on Carboxylate Passivated CdSe Quantum Dots”, Chemistry Research Day, Stony Brook University, Stony Brook, NY, October 2024

Poster – C.V. Hetherington, B. G. Levine, “Taking Inspiration from Molecular Photochemistry for Quantum Dots”, American Conference on Theoretical Chemistry, Chapel Hill, NC, June 2024

Talk – Z. Zaidi, A. Mehmood, B. G. Levine, "Controlling the Excited State Intramolecular Proton Transfer in Oxazoles," American Chemical Society New York Local Section Undergraduate Research Symposium, Brooklyn, NY, May 2024

Talk – A. Mehmood, B. G. Levine, “Simulations of Ultrafast Spectroscopy Observables Using the GPU-accelerated Time-dependent Complete Active Space Configuration Interaction Method,” Virtual International Seminar on Theoretical Advancements (VISTA), Stony Brook, NY, May 2024

Talk – F. Liang, B. G. Levine, “Integrating Quantum Decoherence within Ehrenfest: A Paradigm for Multistage Dynamics”, IACS Research Day, Stony Brook, NY, Apr 2024

Poster – F. Liang, J. Suchan, A. Durden, B. G. Levine, “Integrating Quantum Decoherence within Ehrenfest: A Paradigm for Multistage Dynamics”, IACS Research Day, Stony Brook, NY, Apr 2024

Talk - C.V. Hetherington, B. G. Levine, “Taking Inspiration from Molecular Photochemistry for Quantum Dots: Hot Carrier Cooling via a Cascade of Conical Intersections", BNL-SBU Photochemistry Supergroup, Brookhaven National Laboratory, Upton, NY, April 2024

Poster - C.V. Hetherington, B. G. Levine, "Shining Light on Quantum Dots", IACS Research Day, Stony Brook, NY, April 2024

Poster – Y. You, A. Mehmood, B. G. Levine, “Ultrafast Excited State Dynamics of an Octahedral Chromium(III) Coordination Complex”, IACS Research Day, Stony Brook, NY, Apr 2024

Talk – T. Knoll, B. G. Levine, "Advancing the Simulation of Laser Experiments with GPUs", IACS Research Day, Stony Brook, NY, Apr 2024

Talk – A. Mehmood, B. G. Levine, “Deciphering the Hidden Dance of Excited State Processes: How the Simulated Ultrafast Signals Complement the Experiment” Spring 2024 Meeting of American Chemical Society (ACS), New Orleans, LA, Mar 2024

Presentation – F. Liang, B. G. Levine, “Integrating Quantum Decoherence within Ehrenfest: A Paradigm for Multistage Dynamics”, ACS Spring Meeting, New Orleans, LA, Mar 2024

Poster – F. Liang, J. Suchan, A. Durden, B. G. Levine, “Integrating Quantum Decoherence within Ehrenfest: A Paradigm for Multistage Dynamics”, ACS Spring Meeting, New Orleans, LA, Mar 2024

Talk – T. Knoll, B. G. Levine, "Advancing Electron Dynamics with GPU Accelerated Propagation of LR-TDDFT Amplitudes", ACS Spring Meeting, New Orleans, LA, Mar 2024

Talk – J. Suchan, B. G. Levine, "Exploring long-lived coherences of molecular excited states," ACS Spring 2024, New Orleans, LA, Mar 2024

Talk – J. Suchan, B. G. Levine, "Exploring long-lived coherences of molecular excited states," CECAM Flagship Workshop - Theoretical and Experimental Advances in Atmospheric Photochemistry, Lausanne, Switzerland, Mar 2024

Talk – Y. You, A. Mehmood, B. G. Levine, “Theoretical Study on Photochemical Dynamics of an Excited State Chromium(III) Coordination Complex”, ACS Spring 2024, New Orleans, LA, Mar. 2024

Talk – C.V. Hetherington, B. G. Levine, “Taking inspiration from molecular photochemistry for quantum dots: Hot carrier cooling via a cascade of conical intersections”, American Chemical Society (ACS) Spring 2024 National Meeting, New Orleans, LA, Mar 2024

Talk – C.V. Hetherington, B. G. Levine, “Taking inspiration from molecular photochemistry for quantum dots: Hot carrier cooling via a cascade of conical intersections”, GCS and BSD 1st Annual Student led Research Symposium, Stony Brook University, Stony Brook, NY, March 2024

Poster – C.V. Hetherington, B. G. Levine, “Taking Inspiration from Molecular Photochemistry for Quantum Dots”, GCS and BSD 1st Annual Student led Research Symposium, Stony Brook University, Stony Brook, NY, March 2024

Poster – S. Ohtsuka, A. Mehmood, B. G. Levine, “Theoretical Study of Atomically Precise Gold Nanoclusters,” Stony Brook University Chemistry Research Day, Stony Brook, NY, Dec 2023

Poster – F. Liang, A. Durden, B. G. Levine “Performance of Decoherence-Corrected Ehrenfest Dynamics with Approximate Electronic Eigenspectrum for Dense Manifold Non-adiabatic Nuclear Dynamics Simulations”, Chemistry Research Day, Stony Brook, NY, December 2023

Poster – C. V. Hetherington, B. G. Levine, “Taking Inspiration from Molecular Photochemistry for Quantum Dots”, Chemistry Research Day, Stony Brook University, Stony Brook, NY, December 2023

Poster – J. Suchan, B. G. Levine, “Exploring Long-Lived Coherences of Molecular Excited States,” Stony Brook University Chemistry Research Day, Stony Brook, NY, Dec 2023

Poster – A. Mehmood, M. C. Silfies, T. K. Allison, B. G. Levine, “Simulations of Ultrafast Spectroscopy Observables Using the GPU-accelerated Time-dependent Complete Active Space

Configuration Interaction Method ” Stony Brook University Chemistry Research Day, Stony Brook, NY, Dec 2023

Poster – A. Pereira, A. Mehmood, B. G. Levine, “Unravelling Excited-State Twisting of Amyloid Stain Thioflavin-T: Theoretical Insights” Stony Brook University Chemistry Research Day, Stony Brook, NY, Dec 2023

Poster – T. Knoll, B. G. Levine, “GPU Accelerated Real-Time Propagation of LR-TDDFT Amplitudes for Simulating Electron Dynamics”, Stony Brook University Chemistry Research Day, Stony Brook, NY, Dec 2023

Talk – A. Mehmood, B. G. Levine, “Deciphering the Hidden Dance of Excited State Processes: How Simulated Ultrafast Signals Complement the Experiment,” SBU-BNL Photochemistry Supergroup Meeting, Stony Brook, NY, Nov 2023

Poster – T. Knoll, B. G. Levine, “GPU Accelerated Real-Time Propagation of LR-TDDFT Amplitudes for Simulating Electron Dynamics”, Society for Industrial and Applied Mathematics (SIAM) NY-NJ-PA Annual Meeting, NJIT, Newark, NJ, Oct 2023

Talk – Z. Zaidi, A. Mehmood, B. Levine, "Tuning the Excited State Intramolecular Proton Transfer in Oxazoles", Gulf Coast Undergraduate Research Symposium, Chemistry Division, Rice University, TX, Oct 2023

Talk – F. Liang, A. Durden, B. G. Levine "Incorporating Quantum Decoherence into Ehrenfest – Solution to Multistate Dynamics”, ACS Fall Meeting, San Francisco, CA, Aug 2023

Poster - Z. Zaidi, A. Mehmood, B. Levine, "Tuning the Excited State Intramolecular Proton Transfer in Oxazoles", American Chemical Society Fall 2023 Conference, San Francisco, CA, Aug 2023 *** won ACS COMP Division Undergraduate Poster Award**

Poster – A. Mehmood, B. G. Levine, “Simulations of Ultrafast Spectroscopy Observables Using the GPU-accelerated Time-dependent Complete Active Space Configuration Interaction Method” Annual Meeting of American Chemical Society Fall 2023, San Francisco, CA, Aug 2023

Poster – T. Knoll, B. G. Levine, “Influence of Sulfur Vacancies on Optoelectronic Properties in MoS2 Nanoflakes”, TDDFT School & Workshop: Excited states and dynamics, Rutgers University, Newark, NJ, Jun/Jul 2023

Talk – T. Knoll, B. G. Levine, “Investigating Defects in Semiconductor Nanomaterials for Solar Energy Conversion”, Institute for Advanced Computational Science (IACS) Research Day, Stony Brook, NY, Apr 2023

Poster – F. Liang, B. G. Levine, “Decoherence-Corrected Ehrenfest Dynamics for Multi-state Nonadiabatic Dynamics”, IACS Research Day, Stony Brook, NY, Apr 2023

Talk – C. V. Hetherington, B. G. Levine, “Simulation of Light-Driven Processes in Quantum Dots”, IACS Research Day, IACS Building, Stony Brook, NY, Apr 2023

Poster – Z. Zaidi, A. Mehmood, B. Levine, "Tuning the Excited State Intramolecular Proton Transfer in Oxazoles", Inaugural Physics and Astronomy Undergraduate Research Day, Stony Brook University, Stony Brook, NY, Mar 2023

Talk – C. V. Hetherington, B. G. Levine, “Role of ligands in hot carrier cooling in quantum dots”, American Chemical Society (ACS) Spring 2023 National Meeting, Indiana Convention Center, Indianapolis, IN, USA, Mar 2023

Poster – A. Mehmood, M. C. Silfies, T. K. Allison, B. G. Levine, “First-principles Simulations of Transient Absorption Spectrum,” Stony Brook University Chemistry Research Day, Stony Brook, NY, Oct 2022

Poster – C. V. Hetherington, B. G. Levine, “Role of Ligands in Nonradiative Relaxation Pathways in Quantum Dots,” Stony Brook University Chemistry Research Day, Stony Brook, NY, Oct 2022

Poster – F. Liang, M. P. Esch, B. G. Levine, “Incorporating Decoherence Correction into Ehrenfest Dynamics - Solution to Multistate Dynamics,” Stony Brook University Chemistry Research Day, Stony Brook, NY, Oct 2022

Poster – T. Knoll, B. G. Levine, “Influence of Sulfur Vacancies on Optoelectronic Properties in MoS_2 Nanoflakes,” Stony Brook University Chemistry Research Day, Stony Brook, NY, Oct 2022

Poster – Y. You, B. G. Levine, “Octahedral Chromium(III) Complexes: Electronic Structure and 4T2 State Dynamics,” Stony Brook University Chemistry Research Day, Stony Brook, NY, Oct 2022

Talk – C. V. Hetherington, B. G. Levine, “Hot carrier cooling in quantum dots via a cascade of conical intersections,” National Meeting of the American Chemical Society, Chicago, IL, Aug 2022

Poster – A. Mehmood, B. G. Levine, “First-principles Simulations of Transient Absorption Spectrum,” American Conference on Theoretical Chemistry, Lake Tahoe, CA, July 2022

Poster – F. Liang, M. P. Esch, B. G. Levine, “Incorporating Decoherence Correction into Ehrenfest Dynamics - Solution to Multistate Dynamics,” American Conference on Theoretical Chemistry, Lake Tahoe, CA, July 2022

Poster – C. V. Hetherington, B. G. Levine, “Investigating Hot Carrier Cooling in Quantum Dots,” American Conference on Theoretical Chemistry, Lake Tahoe, CA, July 2022

Poster – F. Liang, M. P. Esch, B. G. Levine, "Incorporating Decoherence Correction into Ehrenfest Dynamics - Solution to Multistate Dynamics," Molecular Interactions and Dynamics Gordon Research Conference, Stonehill College, MA, July 2022

Talk – F. Liang, M. P. Esch, B. G. Levine, "Incorporating Decoherence Correction into Ehrenfest Dynamics - Solution to Multistate Dynamics," Molecular Interactions and Dynamics Gordon Research Symposium, Stonehill College, MA, July 2022

Talk – C. V. Hetherington, B. G. Levine, "Investigating Hot Carrier Cooling in Quantum Dots," IACS Research Day, Stony Brook, NY, Apr 2022

Poster – K. Torres, A. Mehmood, B. G. Levine, "Computational Study of Solvation Effects on the Spectroscopic Properties of Dyes," National Meeting of the American Chemical Society, San Diego, CA, Mar 2022

Talk – A. Mehmood, B. G. Levine, "First-principles Simulations of Transient Absorption Spectra to Probe Ultrafast Proton Transfer Dynamics," National Meeting of the American Chemical Society, online, Mar 2022

Talk – F. Liang, B. G. Levine, M. P. Esch, "Incorporating quantum decoherence into Ehrenfest: Solution to multistate dynamics," National Meeting of the American Chemical Society, online, Aug 2021

Talk – M. P. Esch, B. G. Levine, "Modeling Nonadiabatic Dynamics on Many Electronic States," Virtual International Seminar on Theoretical Advances (VISTA), online, Nov 2020

Talk – A. Durden, B. G. Levine, "Time-Dependent Configuration Interaction," TeraChem Developers' Workship, online, Sept 2020

Talk – M. P. Esch, B. G. Levine, "Towards Modeling Nonadiabatic Dynamics in Dense Manifolds of Electronic States," Midwestern Conference on Theoretical Chemistry, South Bend, IN, May 2019

Poster – F. Liang, B. G. Levine, "Electronic Structure and Dynamics of CdS Nanoparticles with Surface Defects," Midwestern Conference on Theoretical Chemistry, South Bend, IN, May 2019

Poster – W.-T. Peng, B. G. Levine, "Photophysics of Silicon Clusters with Dangling Bond Defects: Different Charged States and Interactions Between Defects," Midwestern Conference on Theoretical Chemistry, South Bend, IN, May 2019

Poster - D. A. Fedorov, B. G. Levine, "Ab Initio Multiple Cloning in Dense Manifolds of Electronic States," Midwestern Conference on Theoretical Chemistry, South Bend, IN, May 2019

Talk – D. A. Fedorov, B. G. Levine, “Ab Initio Multiple Cloning in Dense Manifolds of Electronic States,” National Meeting of the ACS, Orlando, FL, Apr. 2019

Talk – W.-T. Peng, B. S. Fales, B. G. Levine, “Simulating Electron Dynamics of Complex Molecules with Time-Dependent Complete Active Space Configuration Interaction,” National Meeting of the ACS, Orlando, FL, Apr. 2019

Talk – M. P. Esch, B. G. Levine, “Characterization of Conical Intersections in CsPbBr3 Perovskite Surface Models,” National Meeting of the ACS, Boston, MA, August 2018

Talk – D. A. Fedorov, B. G. Levine, “Density at Conical Intersection in Adiabatic Representation: Solution of Schrodinger Equation using Discontinuous Basis Set,” Midwest Theoretical Chemistry Conference, Chicago, IL, June 2018

Poster – M. P. Esch, B. G. Levine, “Characterization of Conical Intersections in CsPbBr3 Perovskite Surface Models,” Midwest Theoretical Chemistry Conference, Chicago, IL, June 2018

Poster – D. Hardwick, B. G. Levine, “Pathways of Nonradiative Recombination in CdSe Semiconductor Materials,” Midwest Theoretical Chemistry Conference, Chicago, IL, June 2018

Poster – W.-T. Peng, B. S. Fales, B. G. Levine, “Simulating Electron Dynamics of Complex Molecules with Time-Dependent Complete Active Space Configuration Interaction,” Midwest Theoretical Chemistry Conference, Chicago, IL, June 2018

Poster – T. Severt, et al., “Experimentally determining the role of each hydrogen site in the formation of H_3O^+ from ethanol,” APS Annual DAMOP Meeting, Ft. Lauderdale, FL, June 2018

Poster – T. Rivera, B. G. Levine, D. Hardwick, “Investigating computational methods to predict organic redox potentials,” National Meeting of the ACS, New Orleans, LA, March 2018

Talk – W.-T. Peng, B. G. Levine, “Conical Intersections Found in Silicon Nanocrystals with a Dangling Bond Defect,” National Meeting of the ACS, Washington, D.C., August 2017

Poster – W.-T. Peng, B. S. Fales, B. G. Levine, “A Time-Dependent Configuration Interaction Method Using Symplectic Integrator,” Midwest Theoretical Chemistry Conference, East Lansing, MI, June 2017

Poster – M. Esch, B. G. Levine, “How Properties of Linear Polyene Minimal Energy Conical Intersections Change with the Chain Length,” Midwest Theoretical Chemistry Conference, East Lansing, MI, June 2017

Poster – D. Metcalf, A. L. Odom, B. G. Levine, “Calculating the Ligand Donor Parameter of Late Transition Metal Compounds,” Midwest Theoretical Chemistry Conference, East Lansing, MI, June 2017

Poster – B. S. Fales, B. G. Levine, "Rank-Reduced Full Configuration Interaction," Midwest Theoretical Chemistry Conference, East Lansing, MI, June 2017

Talk – M. Nairat, M. Webb, M. Esch, V. V. Lozovoy, B. G. Levine, M. Dantus, "Time-resolved signature across the intermolecular response in substituted cyanine dyes," International Symposium on Molecular Spectroscopy, Urbana, IL, June 2017

Talk – B. S. Fales, E. G. Hohenstein, B. G. Levine, "Spin purication and projection methods for determinantal configuration interaction," Midwest Theoretical Chemistry Conference, Pittsburgh, PA, June 2016

Poster – W.-T. Peng, B. S. Fales, B. G. Levine. "Conical intersections in the silicon cluster with a dangling bond defect: the effects of cluster size," Midwest Theoretical Chemistry Conference, Pittsburgh, PA, June 2016

Poster – G. A. Meek, B. G. Levine. "Addressing the second derivative coupling in nonadiabatic molecular dynamics simulations," Midwest Theoretical Chemistry Conference, Pittburgh, PA, June 2016

Talk – G. A. Meek, B. G. Levine. "Addressing the second derivative coupling in nonadiabatic molecular dynamics simulations," National Meeting of the American Chemical Society, San Diego, CA, Mar. 2016

Talk – Y. Shu, B. G. Levine. "Evolutionary design of emitters for organic light-emitting diodes," National Meeting of the American Chemical Society, San Diego, CA, Mar. 2016

Talk – B. S. Fales, B. G. Levine. "Minimum Energy Conical Intersection Characterization Using Complete Active Space Configuration Interaction Wavefunctions," Midwest Theoretical Chemistry Conference, Ann Arbor, MI, June 2015 *** won best contributed talk**

Poster – G. A. Meek, B. G. Levine. "Electronic structure investigation of bipolaron formation and interfacial charge transfer in graphitic carbon nitrides," Midwest Theoretical Chemistry Conference, Ann Arbor, MI, June 2015 *** won best poster**

Talk – G. A. Meek, B. G. Levine. "A Time-Derivative Coupling Scheme for Accurate Electronic State Transition Probabilities in Nonadiabatic Molecular Dynamics," National Meeting of the American Chemical Society, Denver, CO, Mar. 2015

Talk – B. S. Fales, B. G. Levine. "Graphical Processing Unit Acceleration of 'Two-Step' Complete Active Space Configuration Interaction (CASCI) Methods," National Meeting of the American Chemical Society, Denver, CO, Mar. 2015

Poster – Y. Shu, B. G. Levine. "Excited State Dynamics of Oxygen-Containing Defects on the Silicon Surface," American Conference on Theoretical Chemistry, Telluride, CO, July 2014

Poster – B. S. Fales, B. G. Levine. "Novel Approaches for Minimum Energy Conical Intersection Characterization," American Conference on Theoretical Chemistry, Telluride, CO, July 2014

Poster – G. A. Meek, B. G. Levine. "Improved Evaluation of the Time-Derivative Coupling for Accurate Electronic State Transition Probabilities," American Conference on Theoretical Chemistry, Telluride, CO, July 2014

Talk – G. A. Meek, B. G. Levine. "Improved Evaluation of the Time-Derivative Coupling for Accurate Electronic State Transition Probabilities," Midwest Conference on Theoretical Chemistry, Evanston, IL, June 2014

Poster – Y. Shu, B. G. Levine. "Excited State Dynamics of Oxygen-Containing Defects on the Silicon Surface," Midwest Conference on Theoretical Chemistry, Evanston, IL, June 2014

Poster – B. S. Fales, B. G. Levine. "Graphical Processing Unit (GPU) Acceleration of the Improved Virtual Orbital Method," Midwest Conference on Theoretical Chemistry, Evanston, IL, June 2014

Talk – A. Petty, K. Olson, G. Meek, B. G. Levine, T. F. Guarr. "Multielectron transfer processes in strongly coupled bis(pyridinium) systems," National Meeting of the American Chemical Society, Dallas, TX, Mar. 2014

Talk – B. G. Levine, Y. Shu. "Two-step multireference approaches to efficiently model electronic excited states," National Meeting of the American Chemical Society, Dallas, TX, Mar. 2014

Talk – P. Piecuch, J. A. Hansen, M. Ehara, and B. G. Levine. "Utility of new generation of coupled-cluster methods and algorithms in catalytic and structural properties of gold nanoparticles," National Meeting of the American Chemical Society, Dallas, TX, Mar. 2014

Talk – B. G. Levine, Y. Shu, B. S. Fales. "Modeling "picoparticles" to understand non-radiative decay in nanoparticles," National Meeting of the American Chemical Society, Dallas, TX, Mar. 2014

Talk – B. G. Levine "Efficient Multireference Electronic Structure Approach with a Reduced Propensity for Unphysical Wavefunction Symmetry Breaking." National Meeting of the American Chemical Society, New Orleans, LA, Apr. 2013

Talk – B. G. Levine "Nonadiabatic Dynamics of Localized Excitations in Materials: A First Principles Study of the Effect of Oxygen on Silicon Nanoparticle Photoluminescence" American Chemical Society National Meeting, San Diego, CA, Mar. 2012

Talk – A. Baczewski, B. Shanker, S. Mahanti, and B. G. Levine “A Discontinuous Galerkin Framework for Electron Structure Calculations” American Physical Society March Meeting, Boston, MA, Feb. 2012