Stanford

Todd Martinez

David Mulvane Ehrsam and Edward Curtis Franklin Professor of Chemistry and Professor of Photon Science

CONTACT INFORMATION

- **Administrative Contact**

  Maggie Yeung - Administrative Associate

  Email meiyee18@stanford.edu

  Tel (650) 724-7306

Bio

BIO

Theoretical chemist Todd Martínez develops and applies new methods that predict and explain how atoms move in molecules. These methods are used both to design new molecules and to understand the behavior of those that already exist. His research group studies the response of molecules to light (photochemistry) and external force (mechanochemistry). Photochemistry is a critical part of human vision, single-molecule spectroscopy, harnessing solar energy (either to make fuels or electricity), and even organic synthesis. Mechanochemistry represents a novel scheme to promote unusual reactions and potentially to create self-healing materials that resist degradation. The underlying tools embody the full gamut of quantum mechanical effects governing molecules, from chemical bond breaking/formation to electron/proton transfer and electronic excited states.

Professor Martínez was born in Amityville, New York, but spent most of his childhood in Central America and the Caribbean. His chemical curiosity benefitted tremendously from the relaxed safety standards in Central American chemical supply houses, giving him unfettered access to strong acids and bases. When he also became interested in computation, limited or nonexistent computer access forced him to write and debug computer programs on paper. Today, Prof. Martínez combines these interests by working toward theoretical and computational modeling and design of molecules. Martínez received his PhD in chemistry from UCLA in 1994. After postdoctoral study at UCLA and the Hebrew University in Jerusalem, he joined the faculty at the University of Illinois in 1996. In 2009, he joined the faculty at Stanford, where he is now the Ehrsam and Franklin Professor of Chemistry and Professor of Photon Science at SLAC National Accelerator Laboratory. He has received numerous awards for his contributions, including a MacArthur Fellowship (commonly known as the “genius award”). He is currently co-editor of Annual Reviews in Physical Chemistry and an elected member/fellow of the National Academy of Sciences and the American Academy of Arts and Sciences.

Current research in the Martínez lab aims to make molecular modeling both predictive and routine. New approaches to interactive molecular simulation are being developed, in which users interact with a virtual-reality based molecular modeling kit that fully understands quantum mechanics. New techniques to discover heretofore unknown chemical reactions are being developed and tested, exploiting the many efficient methods that the Martínez group has introduced for solving quantum mechanical problems quickly, using a combination of physical/chemical insights and commodity videogaming hardware. For more details, please visit http://mtzweb.stanford.edu.

ACADEMIC APPOINTMENTS

- Professor, Chemistry
- Professor, Photon Science Directorate
- Member, Bio-X
- Principal Investigator, Stanford PULSE Institute

ADMINISTRATIVE APPOINTMENTS

- Diversity Liaison, Department of Chemistry, Stanford University, (2009- present)
- Edward William and Jane Marr Gutgsell Chair in Chemistry, U. Illinois Urbana-Champaisn, (2006-2008)
- Professor of Chemisty, U. Illinois Urbana-Champaign, (1996-2009)

HONORS AND AWARDS

- Fellow, Royal Society of Chemistry (2024)
- Profesor Invitee, Ecole Normale Superieure, Paris (2022)
- Remsen Award, Maryland Section of the ACS (2021)
- Elected Member, National Academy of Sciences (2019)
- Elected Member, International Academy of Quantum Molecular Sciences (2017)
- IAS Benjamin Meeker Visiting Professor, University of Bristol (2017)
- Fellow, American Academy of Arts and Sciences (2011)
- National Security Science and Engineering Faculty Fellow, Department of Defense (2010)
- Distinguished Alumnus, Carol Morgan School, Dominican Republic (2008)
- Fellow, American Association for the Advancement of Science (2006)
- Fellow, American Physical Society (2005)
- MacArthur Fellow, MacArthur Foundation (2005)
- Special Creativity Extension, National Science Foundation (2004)
- University Scholar, U. Illinois Urbana-Champaign (2004)
- Helen Corley Petit Professor, UIUC College of Liberal Arts and Sciences (2002)
- Excellence in Teaching Award, UIUC School of Chemical Sciences (2001)
- Teacher-Scholar Award, Camille & Henry Dreyfus Foundation (2000)
- Beckman Fellow, UIUC Center for Advanced Study (2000)
- Beckman Young Investigator, Arnold and Mabel Beckman Foundation (1999)
- Packard Fellow, David and Lucile Packard Foundation (1999)
- Sloan Fellow, Alfred P. Sloan Foundation (1999)
- CAREER Award, National Science Foundation (1998)
- Research Innovation Award, Research Corporation (1998)

BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Chair, LCLS SLAC/Stanford Search Committee (2012 - present)
- Member, Academic Computing and Information Services Committee, Stanford University (2012 - present)
- Co-chair, Stanford Research Computing Facility Committee (2010 - present)
- Member, Department of Energy Council on Chemical and Biochemical Sciences (2010 - present)

- Chair, SLAC Midrange Computing Committee (2009 - 2009)
- Member, SLAC CIO Search Committee (2009 - 2009)
- Chair, American Chemical Society Theoretical Chemistry Subdivision (2008 - 2009)
- Advisory Board Member, Chemical Physics (2006 - present)
- Advisory Board Member, Physical Chemistry Chemical Physics (2006 - 2011)
- Vice-Chair, American Chemical Society Theoretical Chemistry Subdivision (2006 - 2007)
- Member, Committee of Visitors, Division of Chemistry, National Science Foundation (2004 - 2004)
- Member, Biophysical Society (1996 - present)
- Member, American Chemical Society (1996 - present)

PROGRAM AFFILIATIONS

- Stanford SystemX Alliance

PROFESSIONAL EDUCATION

- Postdoc, UCLA and Hebrew University, Jerusalem , Physical Chemistry (1996)
- PhD, UCLA , Physical Chemistry (1994)
- BS, Calvin College , Chemistry (1989)

LINKS

- The Martinez Group: http://mtzweb.stanford.edu

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

Ab initio molecular dynamics, photochemistry, molecular design, mechanochemistry, graphical processing unit acceleration of electronic structure and molecular dynamics, automated reaction discovery, ultrafast (femtosecond and attosecond) chemical phenomena

Teaching

COURSES

2025-26

- Advanced Physical Chemistry: CHEM 273 (Win)
- Physical Chemistry III: CHEM 175 (Win)

2023-24

- Chemical Principles I: CHEM 31A (Aut)

2022-23

- Chemical Principles I: CHEM 31A (Aut)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Max Moncada Cohen

Postdoctoral Faculty Sponsor

David Juergens, Lixin Lu, Amiel Stephen Paz, Martin Stoehr

Doctoral Dissertation Advisor (AC)

Jan Estrada Pabon, Otto Fajen, Colton Hicks, Garrett Kukier, Ruiyan Wang, Laura Weiler, Harry Zhang, Nancy Zhu

Publications

PUBLICATIONS

- **First-Principles Analysis of Protonation-Induced Electronic Effects in Tetrakis(p-aminophenyl)porphyrin (TAPP).** *The journal of physical chemistry. A*
  Roy, A., Elmanova, A., Jayan, S., Hupfer, M. L., Martínez, T. J., Gryko, D. T., Presselt, M.
  2026
- **Probing the Ultrafast Photodynamics of Dihydroazulene with In Silico Time-Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction.** *The journal of physical chemistry. A*
  Hillers-Bendtsen, A. E., Mikkelsen, K. V., Martinez, T. J.
  2026
- **Complete Active Space Self-Consistent Field with GPU-Accelerated Density Fitting.** *Journal of chemical theory and computation*
  Wang, R., Wang, Y., Lu, L., Hait, D., Martínez, T. J.
  2026
- **Shadow excited state molecular dynamics with the ΔSCF method.** *The Journal of chemical physics*
  Fajen, O. J., Grånäs, O., Martínez, T. J., Niklasson, A. M.
  2026; 164 (9)
- **Accelerating CCSD(T) on Graphical Processing Units (GPUs).** *The journal of physical chemistry. A*
  Fajen, O. J., Kelly, J. E., Hohenstein, E. G., Martinez, T. J.
  2026
- **Robust and Automated Force Field Parameterization Using Validation Sets and Active Learning.** *Journal of chemical theory and computation*
  Curtis, E. R., Martínez, T. J.
  2026
- **Semiempirical Quantum Chemistry in the Age of ab initio Data and Differentiable Programming: I. Differentiable Molecular Orbital Theory.** *Journal of chemical theory and computation*
  Stöhr, M., Martínez, T. J.
  2026
- **Switching and Quantifying the Single-Molecule Mechanochemical Reactivity of Four-Membered Carbocycle Mechanophores within a Single, Photoswitchable Polymer Strand.** *Journal of the American Chemical Society*
  Bowser, B. H., Meisner, J., Benallal, O., Kouznetsova, T. B., Brown, C. L., Hicks, T. J., Martinez, T. J., Craig, S. L.
  2025
- **Accelerating Hartree-Fock and Density Functional Theory Calculations Using Tensor Hypercontraction.** *Journal of chemical theory and computation*
  Hillers-Bendtsen, A. E., Martínez, T. J.
  2025
- **Locating Ab Initio Transition States via Geodesic Construction on Machine-Learned Potential Energy Surfaces.** *Journal of chemical theory and computation*
  Hait, D., Estrada Pabón, J. D., Stöhr, M., Martínez, T. J.
  2025
- **Cascade Mechanochemical Transformation of a Benzobarrelane Polymer.** *Journal of the American Chemical Society*
  Lee, D. C., Flear, E. J., Xu, R., Zheng, K., Martínez, T. J., Xia, Y.
  2025
- **Structural dynamics of laser-ionized cis-stilbene studied by ultrafast electron diffraction** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*
  Saha, S. K., Nunes, J. P. F., Weir, H., Moore, B., Williams, M., Attar, A. R., Luo, D., Ji, F., Heald, L., Hoffmann, M. C., Yang, J., Lin, M., Ware, et al

2025; 58 (17)

- **Lowering the Scaling of Self-Consistent Field Methods by Combining Tensor Hypercontraction and a Density Difference Ansatz.** *The journal of physical chemistry letters*
  Hillers-Bendtsen, A. E., Martinez, T. J.
  2025: 4734-4739
- **Ultrafast Events in Electrocyclic Ring-Opening Reactions.** *Annual review of physical chemistry*
  Liu, Y., Xu, R., Sanchez, D. M., Martínez, T. J., Wolf, T. J.
  2025
- **Initial Conditions for Excited-State Dynamics in Solvated Systems: A Case Study.** *The journal of physical chemistry. B*
  Curtis, E. R., Jones, C. M., Martínez, T. J.
  2025
- **Structure-property relationships for the force-triggered disrotatory ring-opening of cyclobutene** *CHEMICAL SCIENCE*
  Bowser, B. H., Brown, C. L., Meisner, J., Kouznetsova, T. B., Martinez, T. J., Craig, S. L.
  2025
- **Conformational ensembles reveal the origins of serine protease catalysis.** *Science (New York, N.Y.)*
  Du, S., Kretsch, R. C., Parres-Gold, J., Pieri, E., Cruzeiro, V. W., Zhu, M., Pinney, M. M., Yabukarski, F., Schwans, J. P., Martínez, T. J., Herschlag, D.
  2025; 387 (6735): eado5068
- **Photoinduced hydrogen dissociation in thymine predicted by coupled cluster theory.** *Nature communications*
  Kjønstad, E. F., Fajen, O. J., Paul, A. C., Angelico, S., Mayer, D., Gühr, M., Wolf, T. J., Martínez, T. J., Koch, H.
  2024; 15 (1): 10128
- **Fluorination Affects the Force Sensitivity and Nonequilibrium Dynamics of the Mechanochemical Unzipping of Ladderanes.** *Journal of the American Chemical Society*
  Horst, M., Holm, S., Valenta, L., Kouznetsova, T. B., Yang, J., Burns, N. Z., Craig, S. L., Martínez, T. J., Xia, Y.
  2024
- **Extending GPU-accelerated Gaussian integrals in the TeraChem software package to f type orbitals: Implementation and applications.** *The Journal of chemical physics*
  Wang, Y., Hait, D., Johnson, K. G., Fajen, O. J., Zhang, J. H., Guerrero, R. D., Martinez, T. J.
  2024; 161 (17)
- **Attosecond Probing of Coherent Vibrational Dynamics in CBr4.** *The journal of physical chemistry. A*
  Ou, J. H., Hait, D., Rupprecht, P., Beetar, J. E., Martínez, T. J., Leone, S. R.
  2024
- **Prediction of photodynamics of 200 nm excited cyclobutanone with linear response electronic structure and ab initio multiple spawning.** *The Journal of chemical physics*
  Hait, D., Lahana, D., Fajen, O. J., Paz, A. S., Unzueta, P. A., Rana, B., Lu, L., Wang, Y., Kjønstad, E. F., Koch, H., Martínez, T. J.
  2024; 160 (24)
- **Conical Intersection Accessibility Dictates Brightness in Red Fluorescent Proteins.** *Journal of the American Chemical Society*
  Pieri, E., Walker, A. R., Zhu, M., Martínez, T. J.
  2024
- **Photo-induced structural dynamics of o-nitrophenol by ultrafast electron diffraction.** *Physical chemistry chemical physics : PCCP*
  Nunes, J. P., Williams, M., Yang, J., Wolf, T. J., Rankine, C. D., Parrish, R., Moore, B., Wilkin, K., Shen, X., Lin, M. F., Hegazy, K., Li, R., Weathersby, et al
  2024
- **Massively scalable workflows for quantum chemistry: BigChem and ChemCloud.** *The Journal of chemical physics*
  Hicks, C. B., Martinez, T. J.
  2024; 160 (14)
- **QuTree: A tree tensor network package.** *The Journal of chemical physics*
  Ellerbrock, R., Johnson, K. G., Seritan, S., Hoppe, H., Zhang, J. H., Lenzen, T., Weike, T., Manthe, U., Martinez, T. J.

2024; 160 (11)

- **Tensor Hypercontraction of Cluster Perturbation Theory: Quartic Scaling Perturbation Series for the Coupled Cluster Singles and Doubles Ground-State Energies.** *Journal of chemical theory and computation*
  Hillers-Bendtsen, A. E., Mikkelsen, K. V., Martinez, T. J.
  2024
- **Chemical control of excited-state reactivity of the anionic green fluorescent protein chromophore.** *Communications chemistry*
  List, N. H., Jones, C. M., Martinez, T. J.
  2024; 7 (1): 25
- **Predicting the X-ray Absorption Spectrum of Ozone with Single Configuration State Functions.** *Journal of chemical theory and computation*
  Hait, D., Martínez, T. J.
  2024
- **Mechanochemistry of Pterodactylane.** *Journal of the American Chemical Society*
  Horst, M., Meisner, J., Yang, J., Kouznetsova, T. B., Craig, S. L., Martínez, T. J., Xia, Y.
  2023
- **Simulating the Excited-State Dynamics of Polaritons with Ab Initio Multiple Spawning.** *The journal of physical chemistry. A*
  Rana, B., Hohenstein, E. G., Martínez, T. J.
  2023
- **Simulation-guided engineering of split GFPs with efficient β-strand photodissociation.** *Nature communications*
  Shamsudin, Y., Walker, A. R., Jones, C. M., Martínez, T. J., Boxer, S. G.
  2023; 14 (1): 7401
- **Efficient Acceleration of Reaction Discovery in the Ab Initio Nanoreactor: Phenyl Radical Oxidation Chemistry.** *The journal of physical chemistry. A*
  Chang, A. M., Meisner, J., Xu, R., Martínez, T. J.
  2023
- **Sparse adaptive basis set methods for solution of the time dependent Schrodinger equation** *MOLECULAR PHYSICS*
  Thompson, K. C., Martinez, T. J.
  2023
- **Femtosecond Electronic and Hydrogen Structural Dynamics in Ammonia Imaged with Ultrafast Electron Diffraction.** *Physical review letters*
  Champenois, E. G., List, N. H., Ware, M., Britton, M., Bucksbaum, P. H., Cheng, X., Centurion, M., Cryan, J. P., Forbes, R., Gabalski, I., Hegazy, K., Hoffmann, M. C., Howard, et al
  2023; 131 (14): 143001
- **Photo-actuators via epitaxial growth of microcrystal arrays in polymer membranes.** *Nature materials*
  Xu, W., Sanchez, D. M., Raucci, U., Zhou, H., Dong, X., Hu, M., Bardeen, C. J., Martinez, T. J., Hayward, R. C.
  2023
- **First principles reaction discovery: from the Schrodinger equation to experimental prediction for methane pyrolysis.** *Chemical science*
  Xu, R., Meisner, J., Chang, A. M., Thompson, K. C., Martínez, T. J.
  2023; 14 (27): 7447-7464
- **Geometric phase in coupled cluster theory.** *The Journal of chemical physics*
  Williams, D. M., Kjonstad, E. F., Martinez, T. J.
  2023; 158 (21)
- **Rehybridization dynamics into the pericyclic minimum of an electrocyclic reaction imaged in real-time.** *Nature communications*
  Liu, Y., Sanchez, D. M., Ware, M. R., Champenois, E. G., Yang, J., Nunes, J. P., Attar, A., Centurion, M., Cryan, J. P., Forbes, R., Hegazy, K., Hoffmann, M. C., Ji, et al
  2023; 14 (1): 2795
- **Single-Point Extrapolation to the Complete Basis Set Limit through Deep Learning.** *Journal of chemical theory and computation*
  Holm, S., Unzueta, P. A., Thompson, K., Martínez, T. J.
  2023

- **A Nitrogen Out-of-Plane (NOOP) Mechanism for Imine-Based Light-Driven Molecular Motors.** *Journal of the American Chemical Society*
  Liu, L., Fang, W., Martinez, T. J.
  2023
- **SQMBox: Interfacing a semiempirical integral library to modular ab initio electronic structure enables new semiempirical methods.** *The Journal of chemical physics*
  Bannwarth, C., Martinez, T. J.
  2023; 158 (7): 074109
- **2021 JCP Emerging Investigator Special Collection.** *The Journal of chemical physics*
  Ceriotti, M., Jensen, L., Manolopoulos, D. E., Martinez, T., Reichman, D. R., Sciortino, F., Sherrill, C. D., Shi, Q., Vega, C., Wang, L., Weiss, E. A., Zhu, X., Stein, et al
  2023; 158 (6): 060401
- **TeraChem protocol buffers (TCPB): Accelerating QM and QM/MM simulations with a client–server model** *THE JOURNAL OF CHEMICAL PHYSICS*
  Cruzeiro, V. D., Wang, Y., Pieri, E., Hohenstein, E. G., Martínez, T. J.
  2023; 158 (044801)
- **Enhanced Sampling Aided Design of Molecular Photoswitches.** *Journal of the American Chemical Society*
  Raucci, U., Sanchez, D. M., Martinez, T. J., Parrinello, M.
  2022
- **Multinode Multi-GPU Two-Electron Integrals: Code Generation Using the Regent Language.** *Journal of chemical theory and computation*
  Johnson, K. G., Mirchandaney, S., Hoag, E., Heirich, A., Aiken, A., Martinez, T. J.
  2022
- **Steric and Electronic Origins of Fluorescence in GFP and GFP-like Proteins.** *Journal of the American Chemical Society*
  Jones, C. M., List, N. H., Martinez, T. J.
  2022
- **A multi-stage single photochrome system for controlled photoswitching responses.** *Nature chemistry*
  Stricker, F., Sanchez, D. M., Raucci, U., Dolinski, N. D., Zayas, M. S., Meisner, J., Hawker, C. J., Martinez, T. J., Read de Alaniz, J.
  2022
- **InteraChem: Exploring Excited States in Virtual Reality with Ab Initio Interactive Molecular Dynamics.** *Journal of chemical theory and computation*
  Wang, Y., Seritan, S., Lahana, D., Ford, J. E., Valentini, A., Hohenstein, E. G., Martinez, T. J.
  2022
- **Bringing chemical structures to life with augmented reality, machine learning, and quantum chemistry.** *The Journal of chemical physics*
  Sakshuwong, S., Weir, H., Raucci, U., Martinez, T. J.
  2022; 156 (20): 204801
- **Chiral photochemistry of achiral molecules.** *Nature communications*
  Raucci, U., Weir, H., Bannwarth, C., Sanchez, D. M., Martinez, T. J.
  2022; 13 (1): 2091
- **Dissociative electron attachment to 5-bromo-uracil: non-adiabatic dynamics on complex-valued potential energy surfaces.** *Physical chemistry chemical physics : PCCP*
  Cornetta, L. M., Martinez, T. J., Varella, M. T.
  2022
- **Rank-reduced coupled-cluster. III. Tensor hypercontraction of the doubles amplitudes.** *The Journal of chemical physics*
  Hohenstein, E. G., Fales, B. S., Parrish, R. M., Martinez, T. J.
  2022; 156 (5): 054102
- **Interactive Quantum Chemistry Enabled by Machine Learning, Graphical Processing Units, and Cloud Computing.** *Annual review of physical chemistry*
  Raucci, U., Weir, H., Sakshuwong, S., Seritan, S., Hicks, C. B., Vannucci, F., Rea, F., Martínez, T. J.

2022

- **Internal conversion of the anionic GFP chromophore: in and out of the I-twisted S1/S0 conical intersection seam.** *Chemical science*
  List, N. H., Jones, C. M., Martínez, T. J.
  2022; 13 (2): 373-385

- **2020 JCP Emerging Investigator Special Collection.** *The Journal of chemical physics*
  Ceriotti, M., Jensen, L., Manolopoulos, D. E., Martinez, T. J., Michaelides, A., Ogilvie, J. P., Reichman, D. R., Shi, Q., Straub, J. E., Vega, C., Wang, L., Weiss, E., Zhu, et al
  1800; 155 (23): 230401

- **Internal conversion of the anionic GFP chromophore: in and out of the I-twisted S-1/S-0 conical intersection seam** *CHEMICAL SCIENCE*
  List, N. H., Jones, C. M., Martinez, T. J.
  2021

- **Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs.** *The Journal of chemical physics*
  Smith, D. G., Lolinco, A. T., Glick, Z. L., Lee, J., Alenaizan, A., Barnes, T. A., Borca, C. H., Di Remigio, R., Dotson, D. L., Ehlert, S., Heide, A. G., Herbst, M. F., Hermann, et al
  2021; 155 (20): 204801

- **In Silico Discovery of Multistep Chemistry Initiated by a Conical Intersection: The Challenging Case of Donor-Acceptor Stenhouse Adducts.** *Journal of the American Chemical Society*
  Sanchez, D. M., Raucci, U., Martinez, T. J.
  2021

- **InteraChem: Virtual Reality Visualizer for Reactive Interactive Molecular Dynamics** *JOURNAL OF CHEMICAL EDUCATION*
  Seritan, S., Wang, Y., Ford, J. E., Valentini, A., Gold, T., Martinez, T. J.
  2021; 98 (11): 3486-3492

- **Proton Transfer from a Photoacid to a Water Wire: First Principles Simulations and Fast Fluorescence Spectroscopy.** *The journal of physical chemistry. B*
  Walker, A. R., Wu, B., Meisner, J., Fayer, M. D., Martinez, T. J.
  2021

- **Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Hole-Hole Tamm-Dancoff-Approximated Density Functional Theory.** *Journal of chemical theory and computation*
  Hohenstein, E. G., Yu, J. K., Bannwarth, C., List, N. H., Paul, A. C., Folkestad, S. D., Koch, H., Martinez, T. J.
  2021

- **Resolving the ultrafast dynamics of the anionic green fluorescent protein chromophore in water.** *Chemical science*
  Jones, C. M., List, N. H., Martínez, T. J.
  2021; 12 (34): 11347-11363

- **ChemPix: automated recognition of hand-drawn hydrocarbon structures using deep learning.** *Chemical science*
  Weir, H., Thompson, K., Woodward, A., Choi, B., Braun, A., Martínez, T. J.
  2021; 12 (31): 10622-10633

- **Direct observation of ultrafast hydrogen bond strengthening in liquid water.** *Nature*
  Yang, J., Dettori, R., Nunes, J. P., List, N. H., Biasin, E., Centurion, M., Chen, Z., Cordones, A. A., Deponte, D. P., Heinz, T. F., Kozina, M. E., Ledbetter, K., Lin, et al
  2021; 596 (7873): 531-535

- **Understanding the Mechanochemistry of Ladder-Type Cyclobutane Mechanophores by Single Molecule Force Spectroscopy.** *Journal of the American Chemical Society*
  Horst, M., Yang, J., Meisner, J., Kouznetsova, T. B., Martinez, T. J., Craig, S. L., Xia, Y.
  2021

- **A diagrammatic approach for automatically deriving analytical gradients of tensor hyper-contracted electronic structure methods.** *The Journal of chemical physics*
  Song, C., Martinez, T. J., Neaton, J. B.

2021; 155 (2): 024108

- **Resolving the ultrafast dynamics of the anionic green fluorescent protein chromophore in water** *CHEMICAL SCIENCE*
  Jones, C. M., List, N. H., Martinez, T. J.
  2021
- **Flyby reaction trajectories: Chemical dynamics under extrinsic force.** *Science (New York, N.Y.)*
  Liu, Y., Holm, S., Meisner, J., Jia, Y., Wu, Q., Woods, T. J., Martinez, T. J., Moore, J. S.
  2021; 373 (6551): 208-212
- **Unmasking the cis-Stilbene Phantom State via Vacuum Ultraviolet Time-Resolved Photoelectron Spectroscopy and Ab Initio Multiple Spawning.** *The journal of physical chemistry letters*
  Williams, M., Forbes, R., Weir, H., Veyrinas, K., MacDonell, R. J., Boguslavskiy, A. E., Schuurman, M. S., Stolow, A., Martinez, T. J.
  2021: 6363-6369
- **Chemical physics software.** *The Journal of chemical physics*
  Sherrill, C. D., Manolopoulos, D. E., Martinez, T. J., Ceriotti, M., Michaelides, A.
  2021; 155 (1): 010401
- **ChemPix: automated recognition of hand-drawn hydrocarbon structures using deep learning** *CHEMICAL SCIENCE*
  Weir, H., Thompson, K., Woodward, A., Choi, B., Braun, A., Martinez, T. J.
  2021
- **The non-adiabatic nanoreactor: towards the automated discovery of photochemistry** *CHEMICAL SCIENCE*
  Pieri, E., Lahana, D., Chang, A. M., Aldaz, C. R., Thompson, K. C., Martinez, T. J.
  2021
- **The non-adiabatic nanoreactor: towards the automated discovery of photochemistry.** *Chemical science*
  Pieri, E., Lahana, D., Chang, A. M., Aldaz, C. R., Thompson, K. C., Martínez, T. J.
  2021; 12 (21): 7294-7307
- **Electrostatic Control of Photoisomerization in Channelrhodopsin 2.** *Journal of the American Chemical Society*
  Liang, R., Yu, J. K., Meisner, J., Liu, F., Martinez, T. J.
  2021
- **Parallel molecular mechanisms for enzyme temperature adaptation.** *Science (New York, N.Y.)*
  Pinney, M. M., Mokhtari, D. A., Akiva, E., Yabukarski, F., Sanchez, D. M., Liang, R., Doukov, T., Martinez, T. J., Babbitt, P. C., Herschlag, D.
  2021; 371 (6533)
- **Substituent Effects in Mechanochemical Allowed and Forbidden Cyclobutene Ring-Opening Reactions.** *Journal of the American Chemical Society*
  Brown, C. L., Bowser, B. H., Meisner, J., Kouznetsova, T. B., Seritan, S., Martinez, T. J., Craig, S. L.
  2021
- **Nitromethane Decomposition via Automated Reaction Discovery and an Ab Initio Corrected Kinetic Model.** *The journal of physical chemistry. A*
  Ford, J., Seritan, S., Zhu, X., Sakano, M. N., Islam, M. M., Strachan, A., Martinez, T. J.
  2021
- **Transient resonant Auger-Meitner spectra of photoexcited thymine.** *Faraday discussions*
  Wolf, T. J., Paul, A. C., Folkestad, S. D., Myhre, R. H., Cryan, J. P., Berrah, N., Bucksbaum, P. H., Coriani, S., Coslovich, G., Feifel, R., Martinez, T. J., Moeller, S. P., Mucke, et al
  2021
- **Comparing (stochastic-selection) ab initio multiple spawning with trajectory surface hopping for the photodynamics of cyclopropanone, fulvene, and dithiane.** *The Journal of chemical physics*
  Ibele, L. M., Lassmann, Y. n., Martínez, T. J., Curchod, B. F.
  2021; 154 (10): 104110
- **Voice-controlled quantum chemistry.** *Nature computational science*
  Raucci, U., Valentini, A., Pieri, E., Weir, H., Seritan, S., Martínez, T. J.

2021; 1 (1): 42-45

- **GPU acceleration of rank-reduced coupled-cluster singles and doubles.** *The Journal of chemical physics*
  Hohenstein, E. G., Martínez, T. J.
  2021; 155 (18): 184110
- **Voice-controlled quantum chemistry** *NATURE COMPUTATIONAL SCIENCE*
  Raucci, U., Valentini, A., Pieri, E., Weir, H., Seritan, S., Martinez, T. J.
  2021; 1 (1): 42-45
- **Reduced scaling formulation of CASPT2 analytical gradients using the supporting subspace method.** *The Journal of chemical physics*
  Song, C. n., Neaton, J. B., Martínez, T. J.
  2021; 154 (1): 014103
- **A Tribute to Emily A. Carter.** *The journal of physical chemistry. A*
  Zhuang, H. n., Keith, J. n., Martinez, T. n.
  2021; 125 (8): 1669–70
- **Analytical derivatives of the individual state energies in ensemble density functional theory. II. Implementation on graphical processing units (GPUs).** *The Journal of chemical physics*
  Liu, F. n., Filatov, M. n., Martínez, T. J.
  2021; 154 (10): 104108
- **Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the npi* and pipi* Excited States.** *Journal of the American Chemical Society*
  Yu, J. K., Bannwarth, C., Liang, R., Hohenstein, E. G., Martinez, T. J.
  2020
- **An ab initio exciton model for singlet fission.** *The Journal of chemical physics*
  Li, X., Parrish, R. M., Martinez, T. J.
  2020; 153 (18): 184116
- **The Mechanics of the Bicycle Pedal Photoisomerization in Crystalline cis,cis-1,4-Diphenyl-1,3-butadiene.** *The journal of physical chemistry. A*
  Aldaz, C. R., Martinez, T. J., Zimmerman, P. M.
  2020
- **JCP Emerging Investigator Special Collection 2019.** *The Journal of chemical physics*
  Ediger, M. D., Jensen, L., Manolopoulos, D. E., Martinez, T. J., Michaelides, A., Reichman, D. R., Sherrill, C. D., Shi, Q., Straub, J. E., Vega, C., Wang, L., Brigham, E. C., Lian, et al
  2020; 153 (11): 110402
- **Proton Transfer Dynamics in the Aprotic Proton Accepting Solvent 1-Methylimidazole.** *The journal of physical chemistry. B*
  Thomaz, J. E., Walker, A. R., Van Wyck, S. J., Meisner, J., Martinez, T. J., Fayer, M. D.
  2020
- **A multilayer multi-configurational approach to efficiently simulate large-scale circuit-based quantum computers on classical machines.** *The Journal of chemical physics*
  Ellerbrock, R., Martinez, T. J.
  2020; 153 (5): 051101
- **TeraChem: A graphical processing unit-acceleratedelectronic structure package forlarge-scaleab initio molecular dynamics** *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*
  Seritan, S., Bannwarth, C., Fales, B. S., Hohenstein, E. G., Isborn, C. M., Kokkila-Schumacher, S. I. L., Li, X., Liu, F., Luehr, N., Snyder, J. W., Song, C., Titov, A., Ufimtsev, et al
  2020
- **SSAIMS-Stochastic-Selection Ab Initio Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics.** *The journal of physical chemistry. A*
  Curchod, B. F., Glover, W. J., Martinez, T. J.
  2020

- **Strong, Nonresonant Radiation Enhances Cis-Trans Photoisomerization of Stilbene in Solution.** *The journal of physical chemistry. A*
  van den Berg, J. L., Neumann, K. I., Harrison, J. A., Weir, H., Hohenstein, E. G., Martinez, T. J., Zare, R. N.
  2020
- **Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures.** *Journal of chemical theory and computation*
  Fales, B. S., Curtis, E. R., Johnson, K. G., Lahana, D., Seritan, S., Wang, Y., Weir, H., Martinez, T. J., Hohenstein, E. G.
  2020
- **Reduced scaling extended multi-state CASPT2 (XMS-CASPT2) using supporting subspaces and tensor hyper-contraction.** *The Journal of chemical physics*
  Song, C., Martinez, T. J.
  2020; 152 (23): 234113
- **Fast transformations between configuration state function and Slater determinant bases for direct configuration interaction.** *The Journal of chemical physics*
  Fales, B. S., Martinez, T. J.
  2020; 152 (16): 164111
- **Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy** *CHEMICAL SCIENCE*
  List, N. H., Dempwolff, A. L., Dreuw, A., Norman, P., Martinez, T. J.
  2020; 11 (16): 4180–93
- **Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy.** *Chemical science*
  List, N. H., Dempwolff, A. L., Dreuw, A., Norman, P., Martínez, T. J.
  2020; 11 (16): 4180-4193
- **The cascade unzipping of ladderane reveals dynamic effects in mechanochemistry.** *Nature chemistry*
  Chen, Z., Zhu, X., Yang, J., Mercer, J. A., Burns, N. Z., Martinez, T. J., Xia, Y.
  2020
- **Hole-hole Tamm-Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation.** *The Journal of chemical physics*
  Bannwarth, C. n., Yu, J. K., Hohenstein, E. G., Martínez, T. J.
  2020; 153 (2): 024110
- **TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units.** *The Journal of chemical physics*
  Seritan, S. n., Bannwarth, C. n., Fales, B. S., Hohenstein, E. G., Kokkila-Schumacher, S. I., Luehr, N. n., Snyder, J. W., Song, C. n., Titov, A. V., Ufimtsev, I. S., Martínez, T. J.
  2020; 152 (22): 224110
- **Simultaneous observation of nuclear and electronic dynamics by ultrafast electron diffraction.** *Science (New York, N.Y.)*
  Yang, J. n., Zhu, X. n., F Nunes, J. P., Yu, J. K., Parrish, R. M., Wolf, T. J., Centurion, M. n., Gühr, M. n., Li, R. n., Liu, Y. n., Moore, B. n., Niebuhr, M. n., Park, et al
  2020; 368 (6493): 885–89
- **Ab Initio Nonadiabatic Molecular Dynamics with Hole-Hole Tamm-Dancoff Approximated Density Functional Theory.** *Journal of chemical theory and computation*
  Yu, J. K., Bannwarth, C. n., Hohenstein, E. G., Martínez, T. J.
  2020
- **TeraChem Cloud: A High-Performance Computing Service for Scalable Distributed GPU-Accelerated Electronic Structure Calculations.** *Journal of chemical information and modeling*
  Seritan, S. n., Thompson, K. n., Martínez, T. J.
  2020
- **Strictly non-adiabatic quantum control of the acetylene dication using an infrared field.** *The Journal of chemical physics*
  Liekhus-Schmaltz, C. n., Zhu, X. n., McCracken, G. A., Cryan, J. P., Martinez, T. J., Bucksbaum, P. H.
  2020; 152 (18): 184302

- **Intermolecular vibrations mediate ultrafast singlet fission.** *Science advances*
  Duan, H. G., Jha, A. n., Li, X. n., Tiwari, V. n., Ye, H. n., Nayak, P. K., Zhu, X. L., Li, Z. n., Martinez, T. J., Thorwart, M. n., Miller, R. J.
  2020; 6 (38)
- **PySpawn: Software for Nonadiabatic Quantum Molecular Dynamics.** *Journal of chemical theory and computation*
  Fedorov, D. A., Seritan, S. n., Fales, B. S., Martínez, T. J., Levine, B. G.
  2020
- **Efficient Treatment of Large Active Spaces through Multi-GPU Parallel Implementation of Direct Configuration Interaction.** *Journal of chemical theory and computation*
  Fales, B. S., Martínez, T. J.
  2020
- **Putting Photomechanical Switches to Work: An Ab Initio Multiple Spawning Study of Donor-Acceptor Stenhouse Adducts.** *The journal of physical chemistry letters*
  Sanchez, D. M., Raucci, U. n., Ferreras, K. N., Martínez, T. J.
  2020: 7901–7
- **Electronic structure software.** *The Journal of chemical physics*
  Sherrill, C. D., Manolopoulos, D. E., Martínez, T. J., Michaelides, A. n.
  2020; 153 (7): 070401
- **Nonadiabatic Dynamics of Photoexcited cis-Stilbene Using Ab Initio Multiple Spawning.** *The journal of physical chemistry. B*
  Weir, H. n., Williams, M. n., Parrish, R. M., Hohenstein, E. G., Martínez, T. J.
  2020
- **First-Principles Characterization of the Elusive I Fluorescent State and the Structural Evolution of Retinal Protonated Schiff Base in Bacteriorhodopsin.** *Journal of the American Chemical Society*
  Yu, J. K., Liang, R., Liu, F., Martinez, T. J.
  2019
- **Rank reduced coupled cluster theory. II. Equation-of-motion coupled-cluster singles and doubles.** *The Journal of chemical physics*
  Hohenstein, E. G., Zhao, Y., Parrish, R. M., Martinez, T. J.
  2019; 151 (16): 164121
- **Computational Discovery of the Origins of Life.** *ACS central science*
  Meisner, J., Zhu, X., Martinez, T. J.
  2019; 5 (9): 1493–95
- **Reaction Dynamics of Cyanohydrins with Hydrosulfide in Water.** *The journal of physical chemistry. A*
  Valleau, S., Martinez, T. J.
  2019
- **Diffractive imaging of dissociation and ground-state dynamics in a complex molecule** *PHYSICAL REVIEW A*
  Wilkin, K. J., Parrish, R. M., Yang, J., Wolf, T. J. A., Nunes, J. F., Guehr, M., Li, R., Shen, X., Zheng, Q., Wang, X., Martinez, T. J., Centurion, M.
  2019; 100 (2)
- **Disentangling conical intersection and coherent molecular dynamics in methyl bromide with attosecond transient absorption spectroscopy.** *Nature communications*
  Timmers, H., Zhu, X., Li, Z., Kobayashi, Y., Sabbar, M., Hollstein, M., Reduzzi, M., Martinez, T. J., Neumark, D. M., Leone, S. R.
  2019; 10 (1): 3133
- **Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver.** *Physical review letters*
  Parrish, R. M., Hohenstein, E. G., McMahon, P. L., Martínez, T. J.
  2019; 122 (23): 230401
- **Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver** *PHYSICAL REVIEW LETTERS*
  Parrish, R. M., Hohenstein, E. G., McMahon, P. L., Martinez, T. J.
  2019; 122 (23)

- **Nonadiabatic Photodynamics of Retinal Protonated Schiff Base in Channelrhodopsin 2** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Liang, R., Liu, F., Martinez, T. J.
  2019; 10 (11): 2862–68
- **On combining the conductor-like screening model and optimally tuned range-separated hybrid density functionals.** *The Journal of chemical physics*
  Sachse, T., Martinez, T. J., Presselt, M.
  2019; 150 (17): 174117
- **Ab initio Computation of Rotationally-Averaged Pump-Probe X-ray and Electron Diffraction Signals** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Parrish, R. M., Martinez, T. J.
  2019; 15 (3): 1523-1537
- **Sub-Femtosecond Stark Control of Molecular Photoexcitation with Near Single-Cycle Pulses** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Mignolet, B., Curchod, B. F. E., Remacle, F., Martinez, T. J.
  2019; 10 (4): 742-747
- **Ab Initio Computation of Rotationally-Averaged Pump-Probe X-ray and Electron Diffraction Signals.** *Journal of chemical theory and computation*
  Parrish, R. M., Martinez, T. J.
  2019
- **Multicolor Mechanochromism of a Polymer/Silica Composite with Dual Distinct Mechanophores** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Kosuge, T., Zhu, X., Lau, V. M., Aoki, D., Martinez, T. J., Moore, J. S., Otsuka, H.
  2019; 141 (5): 1898-1902
- **Sub-Femtosecond Stark Control of Molecular Photoexcitation with Near Single-Cycle Pulses.** *The journal of physical chemistry letters*
  Mignolet, B., Curchod, B. F., Remacle, F., Martinez, T. J.
  2019: 742–47
- **Multicolor Mechanochromism of a Polymer/Silica Composite with Dual Distinct Mechanophores.** *Journal of the American Chemical Society*
  Kosuge, T., Zhu, X., Lau, V. M., Aoki, D., Martinez, T. J., Moore, J. S., Otsuka, H.
  2019
- **Exploiting graphical processing units to enable quantum chemistry calculation of large solvated molecules with conductor-like polarizable continuum models**
  Liu, F., Sanchez, D. M., Kulik, H. J., Martinez, T. J.
  WILEY.2019
- **Geodesic interpolation for reaction pathways.** *The Journal of chemical physics*
  Zhu, X. n., Thompson, K. C., Martínez, T. J.
  2019; 150 (16): 164103
- **Relaxation Dynamics of Hydrated Thymine, Thymidine, and Thymidine Monophosphate Probed by Liquid Jet Time-Resolved Photoelectron Spectroscopy.** *The journal of physical chemistry. A*
  Erickson, B. A., Heim, Z. N., Pieri, E. n., Liu, E. n., Martinez, T. J., Neumark, D. M.
  2019
- **Imaging the ring opening reaction of 1,3-cyclohexadiene with MeV ultrafast electron diffraction**
  Wolf, T. J. A., Yang, J., Sanchez, D. M., Nunes, J. F., Parrish, R. M., Shen, X., Centurion, M., Coffee, R., Gyan, J. P., Guhr, M., Kareem, H., Kirrander, A., Li, et al
  edited by Cerullo, G., Ogilvie, J., Kartner, F., Khalil, M., Li, R.
  E D P SCIENCES.2019
- **Nonadiabatic Photodynamics of Retinal Protonated Schiff Base in Channelrhodopsin 2.** *The journal of physical chemistry letters*
  Liang, R. n., Liu, F. n., Martínez, T. J.
  2019: 2862–68

- **Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy.** *The journal of physical chemistry. A*
  Wolf, T. J., Parrish, R. M., Myhre, R. H., Martínez, T. J., Koch, H. n., Gühr, M. n.
  2019

- **Perturbation of Short Hydrogen Bonds in Photoactive Yellow Protein via Noncanonical Amino Acid Incorporation.** *The journal of physical chemistry. B*
  Thomson, B. n., Both, J. n., Wu, Y. n., Parrish, R. M., Martínez, T. J., Boxer, S. G.
  2019

- **Rank reduced coupled cluster theory. I. Ground state energies and wavefunctions.** *The Journal of chemical physics*
  Parrish, R. M., Zhao, Y. n., Hohenstein, E. G., Martínez, T. J.
  2019; 150 (16): 164118

- **Ab Initio Prediction of Fluorescence Lifetimes Involving Solvent Environments by Means of COSMO and Vibrational Broadening** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Preiss, J., Kage, D., Hoffmann, K., Martinez, T. J., Resch-Genger, U., Presselt, M.
  2018; 122 (51): 9813–20

- **Structural Coupling Throughout the Active Site Hydrogen Bond Networks of Ketosteroid Isomerase and Photoactive Yellow Protein** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Pinney, M. M., Natarajan, A., Yabukarski, F., Sanchez, D. M., Liu, F., Liang, R., Doukov, T., Schwans, J. P., Martinez, T. J., Herschlag, D.
  2018; 140 (31): 9827–43

- **Reduced scaling CASPT2 using supporting subspaces and tensor hyper-contraction.** *The Journal of chemical physics*
  Song, C., Martinez, T. J.
  2018; 149 (4): 044108

- **Reduced scaling CASPT2 using supporting subspaces and tensor hyper-contraction** *JOURNAL OF CHEMICAL PHYSICS*
  Song, C., Martinez, T. J.
  2018; 149 (4)

- **Imaging CF3I conical intersection and photodissociation dynamics with ultrafast electron diffraction.** *Science (New York, N.Y.)*
  Yang, J., Zhu, X., Wolf, T. J., Li, Z., Nunes, J. P., Coffee, R., Cryan, J. P., Gühr, M., Hegazy, K., Heinz, T. F., Jobe, K., Li, R., Shen, et al
  2018; 361 (6397): 64-67

- **A Program for Automatically Predicting Supramolecular Aggregates and Its Application to Urea and Porphin** *JOURNAL OF COMPUTATIONAL CHEMISTRY*
  Sachse, T., Martinez, T. J., Dietzek, B., Presselt, M.
  2018; 39 (13): 763–72

- **Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. II. Ab initio multiple spawning simulations** *JOURNAL OF CHEMICAL PHYSICS*
  Glover, W. J., Mori, T., Schuurman, M. S., Boguslavskiy, A. E., Schalk, O., Stolow, A., Martinez, T. J.
  2018; 148 (16): 164303

- **Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. I. Time-resolved photoelectron-photoion coincidence spectroscopy** *JOURNAL OF CHEMICAL PHYSICS*
  Boguslavskiy, A. E., Schalk, O., Gador, N., Glover, W. J., Mori, T., Schultz, T., Schuurman, M. S., Martinez, T. J., Stolow, A.
  2018; 148 (16): 164302

- **Ab Initio Nonadiabatic Quantum Molecular Dynamics** *CHEMICAL REVIEWS*
  Curchod, B. F. E., Martinez, T. J.
  2018; 118 (7): 3305–36

- **Mixed quantum-classical electrodynamics: Understanding spontaneous decay and zero-point energy** *PHYSICAL REVIEW A*
  Li, T. E., Nitzan, A., Sukharev, M., Martinez, T., Chen, H., Subotnik, J. E.
  2018; 97 (3)

- **Large-Scale Functional Group Symmetry-Adapted Perturbation Theory on Graphical Processing Units** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*

Parrish, R. M., Thompson, K. C., Martinez, T. J.
2018; 14 (3): 1737–53

- **Rational Protein Design via Structure-Energetics-Function Relationships in the Photoactive Yellow Protein (PYP) Model System**
  Both, J. H., Parrish, R. M., Martinez, T. J., Boxer, S. G.
  CELL PRESS.2018: 410A

- **Nonadiabatic Ab Initio Molecular Dynamics with the Floating Occupation Molecular Orbital-Complete Active Space Configuration Interaction Method** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Hollas, D., Sistik, L., Hohenstein, E. G., Martinez, T. J., Slavicek, P.
  2018; 14 (1): 339–50

- **Large Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction.** *Journal of chemical theory and computation*
  Fales, B. S., Seritan, S. n., Settje, N. F., Levine, B. G., Koch, H. n., Martínez, T. J.
  2018

- **Imaging CF3I conical intersection and photodissociation dynamics with ultrafast electron diffraction** *Science*
  Yang, J., Zhu, X., Wolf, T. J., Li, Z., Nunes, J. F., Coffee, R., Cryan, J. P., Gühr, M., Hegazy, K., Heinz, T. F., Jobe, K., Li, R., Shen, et al
  2018; 361 (6397): 64-67

- **The Quality of the Embedding Potential Is Decisive for Minimal Quantum Region Size in Embedding Calculations: The Case of the Green Fluorescent Protein** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Nabo, L. J., Olsen, J., Martinez, T. J., Kongsted, J.
  2017; 13 (12): 6230–36

- **Pomeranz-Fritsch Synthesis of Isoquinoline: Gas-Phase Collisional Activation Opens Additional Reaction Pathways** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Banerjee, S., Liu, F., Sanchez, D. M., Martinez, T. J., Zare, R. N.
  2017; 139 (41): 14352–55

- **Ultrafast isomerization in acetylene dication after carbon K-shell ionization** *NATURE COMMUNICATIONS*
  Li, Z., Inhester, L., Liekhus-Schmaltz, C., Curchod, B. F. E., Snyder, J. W., Medvedev, N., Cryan, J., Osipov, T., Pabst, S., Vendrell, O., Bucksbaum, P., Martinez, T. J.
  2017; 8: 453

- **The Spin-Flip Variant of the Algebraic-Diagrammatic Construction Yields the Correct Topology of s(1)/S-0 Conical Intersections** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Lefrancois, D., Tuna, D., Martinez, T. J., Dreuw, A.
  2017; 13 (9): 4436–41

- **Understanding the mechanochemistry of molecular ladders**
  Chen, Z., Chen, L., Mercer, J., Zhu, X., Martinez, T., Burns, N., Xia, Y.
  AMER CHEMICAL SOC.2017

- **Mechanochemical unzipping of insulating polyladderene to semiconducting polyacetylene.** *Science (New York, N.Y.)*
  Chen, Z., Mercer, J. A., Zhu, X., Romaniuk, J. A., Pfattner, R., Cegelski, L., Martinez, T. J., Burns, N. Z., Xia, Y.
  2017; 357 (6350): 475-479

- **An Ab Initio Exciton Model Including Charge-Transfer Excited States** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Li, X., Parrish, R. M., Liu, F., Schumacher, S., Martinez, T. J.
  2017; 13 (8): 3493–3504

- **Analytical derivatives of the individual state energies in ensemble density functional theory method. I. General formalism** *JOURNAL OF CHEMICAL PHYSICS*
  Filatov, M., Liu, F., Martinez, T. J.
  2017; 147 (3): 034113

- **Observing Femtosecond Fragmentation Using Ultrafast X-ray-Induced Auger Spectra** *APPLIED SCIENCES-BASEL*
  Wolf, T. J. A., Holzmeier, F., Wagner, I., Berrah, N., Bostedt, C., Bozek, J., Bucksbaum, P., Coffee, R., Cryan, J., Farrell, J., Feifel, R., Martinez, T. J., McFarland, et al
  2017; 7 (7)

- **a-CASSCF: An Efficient, Empirical Correction for SA-CASSCF To Closely Approximate MS-CASPT2 Potential Energy Surfaces.** *journal of physical chemistry letters*
  Snyder, J. W., Parrish, R. M., Martínez, T. J.
  2017; 8 (11): 2432-2437
- **A direct-compatible formulation of the coupled perturbed complete active space self-consistent field equations on graphical processing units** *JOURNAL OF CHEMICAL PHYSICS*
  Snyder, J. W., Fales, B. S., Hohenstein, E. G., Levine, B. G., Martinez, T. J.
  2017; 146 (17)
- **Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Wang, L., McKiernan, K. A., Gomes, J., Beauchamp, K. A., Head-Gordon, T., Rice, J. E., Swope, W. C., Martinez, T. J., Pande, V. S.
  2017; 121 (16): 4023-4039
- **Atomistic non-adiabatic dynamics of the LH2 complex with a GPU-accelerated ab initio exciton model.** *Physical chemistry chemical physics : PCCP*
  Sisto, A., Stross, C., van der Kamp, M. W., O'Connor, M., McIntosh-Smith, S., Johnson, G. T., Hohenstein, E. G., Manby, F. R., Glowacki, D. R., Martinez, T. J.
  2017
- **Reduced-order formulation of multi-reference perturbation theory via tensor hyper-contraction**
  Song, C., Martinez, T.
  AMER CHEMICAL SOC.2017
- **Development of pressure-sensitive amorphous materials bearing TCAQ motifs**
  Ren, Y., Lee, S., Christensen, J., Plotnikov, N., Burgess, M., Martinez, T., Dlott, D., Moore, J.
  AMER CHEMICAL SOC.2017
- **GPU-accelerated state-averaged complete active space self-consistent field and derivative methods enable accurate, large-scale nonadiabatic dynamics simulations**
  Snyder, J., Hohenstein, E., Curchod, B., Fales, B., Parrish, R., Martinez, T.
  AMER CHEMICAL SOC.2017
- **Large-scale selected configuration interaction based on a Davidson-Liu flow**
  Parrish, R., Martinez, T.
  AMER CHEMICAL SOC.2017
- **Atomic orbital-based SOS-MP2 with tensor hypercontraction. II. Local tensor hypercontraction.** *journal of chemical physics*
  Song, C., Martínez, T. J.
  2017; 146 (3): 034104-?
- **Ab Initio Multiple Spawning Photochemical Dynamics of DMABN Using GPUs** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Curchod, B. F., Sisto, A., Martinez, T. J.
  2017; 121 (1): 265-276
- **Crossing conditions in coupled cluster theory.** *The Journal of chemical physics*
  Kjønstad, E. F., Myhre, R. H., Martínez, T. J., Koch, H. n.
  2017; 147 (16): 164105
- **Mechanochemical unzipping of insulating polyladderene to semiconducting polyacetylene** *Science*
  Chen, Z., Mercer, J. A., Zhu, X., Romaniuk, J. A., Pfattner, R., Cegelski, L., Martinez, T. J., Burns, N. Z., Xia, Y.
  2017; 357 (6350): 475-479
- **Description of ground and excited electronic states by ensemble density functional method with extended active space.** *The Journal of chemical physics*
  Filatov, M. n., Martínez, T. J., Kim, K. S.
  2017; 147 (6): 064104
- **Analytical gradients for tensor hyper-contracted MP2 and SOS-MP2 on graphical processing units.** *The Journal of chemical physics*
  Song, C. n., Martínez, T. J.

2017; 147 (16): 161723

- **Ab Initio Reactive Computer Aided Molecular Design.** *Accounts of chemical research*
  Martínez, T. J.
  2017; 50 (3): 652–56
- **Absorption and Fluorescence Features of an Amphiphilic meso-Pyrimidinylcorrole: Experimental Study and Quantum Chemical Calculations.** *The journal of physical chemistry. A*
  Preiß, J. n., Herrmann-Westendorf, F. n., Ngo, T. H., Martínez, T. n., Dietzek, B. n., Hill, J. P., Ariga, K. n., Kruk, M. M., Maes, W. n., Presselt, M. n.
  2017; 121 (45): 8614–24
- **Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs** *JOURNAL OF CHEMICAL PHYSICS*
  Filatov, M., Liu, F., Kim, K. S., Martinez, T. J.
  2016; 145 (24)
- **Communication: XFAIMS-eXternal Field Ab Initio Multiple Spawning for electron-nuclear dynamics triggered by short laser pulses** *JOURNAL OF CHEMICAL PHYSICS*
  Mignolet, B., Curchod, B. F., Martinez, T. J.
  2016; 145 (19)
- **How Large Should the QM Region Be in QM/MM Calculations? The Case of Catechol O-Methyltransferase.** *journal of physical chemistry. B*
  Kulik, H. J., Zhang, J., Klinman, J. P., Martínez, T. J.
  2016: -?
- **Rich Athermal Ground-State Chemistry Triggered by Dynamics through a Conical Intersection.** *Angewandte Chemie (International ed. in English)*
  Mignolet, B., Curchod, B. F., Martínez, T. J.
  2016
- **Pressure-Induced Neutral-to-Ionic Transition in an Amorphous Organic Material** *CHEMISTRY OF MATERIALS*
  Ren, Y., Lee, S., Christensen, J. M., Plotnikov, N. V., Burgess, M., Martinez, T. J., Dlott, D. D., Moore, J. S.
  2016; 28 (18): 6446-6449
- **Toward fully quantum modelling of ultrafast photodissociation imaging experiments. Treating tunnelling in the ab initio multiple cloning approach.** *Faraday discussions*
  Makhov, D. V., Martinez, T. J., Shalashilin, D. V.
  2016: -?
- **Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
  Filatov, M., Martinez, T. J., Kim, K. S.
  2016; 18 (31): 21040-21050
- **Ground and excited state ab initio molecular dynamics using graphical processing units**
  Martinez, T.
  AMER CHEMICAL SOC.2016
- **Molecular Origin of Mechanical Sensitivity of the Reaction Rate in Anthracene Cyclophane Isomerization Reveals Structural Motifs for Rational Design of Mechanophores** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Plotnikov, N. V., Martinez, T. J.
  2016; 120 (32): 17898-17908
- **Adapting DFT+U for the Chemically Motivated Correction of Minimal Basis Set Incompleteness.** *journal of physical chemistry. A*
  Kulik, H. J., Seelam, N., Mar, B. D., Martínez, T. J.
  2016; 120 (29): 5939-5949
- **Comment on "Positive semidefinite tensor factorizations of the two-electron integral matrix for low-scaling ab initio electronic structure" [J. Chem. Phys. 143, 064103 (2015)].** *journal of chemical physics*
  Parrish, R. M., Hohenstein, E. G., Martínez, T. J.
  2016; 145 (2): 027101-?

- **GPU-Accelerated State-Averaged Complete Active Space Self-Consistent Field Interfaced with Ab Initio Multiple Spawning Unravels the Photodynamics of Provitamin D-3** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Snyder, J. W., Curchod, B. F., Martinez, T. J.
  2016; 7 (13): 2444-2449
- **"Balancing" the Block Davidson-Liu Algorithm** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Parrish, R. M., Hohenstein, E. G., Martinez, T. J.
  2016; 12 (7): 3003-3007
- **Correction to "Toward Nonadiabatic Dynamics of Multichromophore Complexes: A Scalable GPU-Accelerated Exciton Framework.** *Accounts of chemical research*
  Sisto, A., Glowacki, D. R., Martinez, T. J.
  2016; 49 (6): 1331-?
- **Atomic orbital-based SOS-MP2 with tensor hypercontraction. I. GPU-based tensor construction and exploiting sparsity** *JOURNAL OF CHEMICAL PHYSICS*
  Song, C., Martinez, T. J.
  2016; 144 (17)
- **Communication: A difference density picture for the self-consistent field ansatz.** *journal of chemical physics*
  Parrish, R. M., Liu, F., Martínez, T. J.
  2016; 144 (13): 131101-?
- **Communication: GAIMS-Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes** *JOURNAL OF CHEMICAL PHYSICS*
  Curchod, B. F., Rauer, C., Marquetand, P., Gonzalez, L., Martinez, T. J.
  2016; 144 (10)
- **Systematic improvement of intramolecular parameters for protein force fields from quantum chemistry data**
  Wang, L., Beauchamp, K., Swope, W., Rice, J., Head-Gordon, T., Martinez, T., Pande, V.
  AMER CHEMICAL SOC.2016
- **Development of organic charge transfer complexes for shock wave energy dissipation (SWED)**
  Ren, Y., Lee, S., Christensen, J., Shaw, W., Plotnikov, N., Martinez, T., Dlott, D., Moore, J.
  AMER CHEMICAL SOC.2016
- **Automated code engine for generation and optimization of electronic integrals on graphics processing hardware**
  Song, C., Wang, L., Martinez, T.
  AMER CHEMICAL SOC.2016
- **Dynamical Correlation Effects on Photoisomerization: Ab Initio Multiple Spawning Dynamics with MS-CASPT2 for a Model trans-Protonated Schiff Base** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Liu, L., Liu, J., Martinez, T. J.
  2016; 120 (8): 1940-1949
- **Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Wang, L., McGibbon, R. T., Pande, V. S., Martinez, T. J.
  2016; 12 (2): 638-649
- **Automated Code Engine for Graphical Processing Units: Application to the Effective Core Potential Integrals and Gradients.** *Journal of chemical theory and computation*
  Song, C., Wang, L. P., Martínez, T. J.
  2016; 12 (1): 92-106
- **Automated Code Engine for Graphical Processing Units: Application to the Effective Core Potential Integrals and Gradients** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Song, C., Wang, L., Martinez, T. J.
  2016; 12 (1): 92-106
- **Evidence of Hydrogen Migration rather than Isomerization in the Acetylene Dication**
  Liekhus-Schmaltz, C. E., Li, Z., Petrovic, V., Martinez, T., Bucksbaum, P. H., IEEE

IEEE.2016

- **Catch and Release: Orbital Symmetry Guided Reaction Dynamics from a Freed "Tension Trapped Transition State"** *JOURNAL OF ORGANIC CHEMISTRY*
  Wang, J., Ong, M. T., Kouznetsova, T. B., Lenhardt, J. M., Martinez, T. J., Craig, S. L.
  2015; 80 (23): 11773-11778
- **An atomic orbital-based formulation of analytical gradients and nonadiabatic coupling vector elements for the state-averaged complete active space self-consistent field method on graphical processing units** *JOURNAL OF CHEMICAL PHYSICS*
  Snyder, J. W., Hohenstein, E. G., Luehr, N., Martinez, T. J.
  2015; 143 (15)
- **Ab initio interactive molecular dynamics on graphical processing units (GPUs).** *Journal of chemical theory and computation*
  Luehr, N., Jin, A. G., Martínez, T. J.
  2015; 11 (10): 4536-44
- **Ab Initio Interactive Molecular Dynamics on Graphical Processing Units (GPUs)** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Luehr, N., Jin, A. G., Martinez, T. J.
  2015; 11 (10): 4536-4544
- **Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces** *JOURNAL OF CHEMICAL PHYSICS*
  Michaelides, A., Martinez, T. J., Alavi, A., Kresse, G., Manby, F. R.
  2015; 143 (10)
- **Ab initio multiple spawning on laser-dressed states: a study of 1,3-cyclohexadiene photoisomerization via light-induced conical intersections** *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*
  Kim, J., Tao, H., Martinez, T. J., Bucksbaum, P.
  2015; 48 (16)
- **Energy refinement of reactive molecular dynamics pathways**
  Wang, L., McGibbon, R., Pande, V., Martinez, T.
  AMER CHEMICAL SOC.2015
- **Molecular dynamics investigation of deeply supercooled water using a direct polarization model**
  Wang, L., Schwantes, C., Lane, T., Sellberg, J., Nilsson, A., Martinez, T., Pande, V.
  AMER CHEMICAL SOC.2015
- **Quantum Chemistry for Solvated Molecules on Graphical Processing Units Using Polarizable Continuum Models.** *Journal of chemical theory and computation*
  Liu, F., Luehr, N., Kulik, H. J., Martínez, T. J.
  2015; 11 (7): 3131-44
- **Tensor Hypercontraction Second-Order Møller-Plesset Perturbation Theory: Grid Optimization and Reaction Energies.** *Journal of chemical theory and computation*
  Schumacher, S. I., Hohenstein, E. G., Parrish, R. M., Wang, L. P., Martínez, T. J.
  2015; 11 (7): 3042-52
- **Efficient implementation of effective core potential integrals and gradients on graphical processing units.** *journal of chemical physics*
  Song, C., Wang, L., Sachse, T., Preiss, J., Presselt, M., Martínez, T. J.
  2015; 143 (1): 014114-?
- **Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units.** *journal of chemical physics*
  Hohenstein, E. G., Bouduban, M. E., Song, C., Luehr, N., Ufimtsev, I. S., Martínez, T. J.
  2015; 143 (1): 014111-?
- **Origin of the Individual Basicity of Corrole NH-Tautomers: A Quantum Chemical Study on Molecular Structure and Dynamics, Kinetics, and Thermodynamics** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Beenken, W., Maes, W., Kruk, M., Martinez, T., Presselt, M.
  2015; 119 (26): 6875-6883

- **Quantum Chemistry for Solvated Molecules on Graphical Processing Units Using Polarizable Continuum Models** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Liu, F., Luehr, N., Kulik, H. J., Martinez, T. J.
  2015; 11 (7): 3131-3144

- **Tensor Hypercontraction Second-Order Moller-Plesset Perturbation Theory: Grid Optimization and Reaction Energies** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Schumacher, S. I., Hohenstein, E. G., Parrish, R. M., Wang, L., Martinez, T. J.
  2015; 11 (7): 3042-3052

- **Mediation of donor-acceptor distance in an enzymatic methyl transfer reaction** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Zhang, J., Kulik, H. J., Martinez, T. J., Klinman, J. P.
  2015; 112 (26): 7954-7959

- **An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units** *JOURNAL OF CHEMICAL PHYSICS*
  Hohenstein, E. G., Luehr, N., Ufimtsev, I. S., Martinez, T. J.
  2015; 142 (22)

- **How Does Peripheral Functionalization of Ruthenium(II)-Terpyridine Complexes Affect Spatial Charge Redistribution after Photoexcitation at the Franck-Condon Point?** *CHEMPHYSCHEM*
  Preiss, J., Jaeger, M., Rau, S., Dietzek, B., Popp, J., Martinez, T., Presselt, M.
  2015; 16 (7): 1395-1404

- **Determination of Hydrogen Bond Structure in Water versus Aprotic Environments To Test the Relationship Between Length and Stability** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Sigala, P. A., Ruben, E. A., Liu, C. W., Piccoli, P. M., Hohenstein, E. G., Martinez, T. J., Schultz, A. J., Herschlag, D.
  2015; 137 (17): 5730-5740

- **Inducing and quantifying forbidden reactivity with single-molecule polymer mechanochemistry** *NATURE CHEMISTRY*
  Wang, J., Kouznetsova, T. B., Niu, Z., Ong, M. T., Klukovich, H., Rheingold, A. L., Martinez, T. J., Craig, S. L.
  2015; 7 (4): 323-327

- **Understanding mechanochemistry from first principles**
  Martinez, T.
  AMER CHEMICAL SOC.2015

- **Ab initio exciton model for nonadiabatic dynamics of multichromophoric systems on GPUs**
  Sisto, A., Glowacki, D., Martinez, T.
  AMER CHEMICAL SOC.2015

- **Ab initio multiple cloning simulations of pyrrole photodissociation: TKER spectra and velocity map imaging.** *Physical chemistry chemical physics*
  Makhov, D. V., Saita, K., Martinez, T. J., Shalashilin, D. V.
  2015; 17 (5): 3316-3325

- **Direct QM/MM Excited-State Dynamics of Retinal Protonated Schiff Base in Isolation and Methanol Solution.** *journal of physical chemistry. B*
  Punwong, C., Owens, J., Martínez, T. J.
  2015; 119 (3): 704-714

- **Ultrafast isomerization initiated by X-ray core ionization.** *Nature communications*
  Liekhus-Schmaltz, C. E., Tenney, I., Osipov, T., Sanchez-Gonzalez, A., Berrah, N., Boll, R., Bomme, C., Bostedt, C., Bozek, J. D., Carron, S., Coffee, R., Devin, J., Erk, et al
  2015; 6: 8199-?

- **Ultrafast isomerization initiated by X-ray core ionization.** *Nature communications*
  Liekhus-Schmaltz, C. E., Tenney, I., Osipov, T., Sanchez-Gonzalez, A., Berrah, N., Boll, R., Bomme, C., Bostedt, C., Bozek, J. D., Carron, S., Coffee, R., Devin, J., Erk, et al
  2015; 6: 8199-?

- **Quantum chemical insights into the dependence of porphyrin basicity on the meso-aryl substituents: thermodynamics, buckling, reaction sites and molecular flexibility** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
  Presselt, M., Dehaen, W., Maes, W., Klamt, A., Martinez, T., Beenken, W. J., Kruk, M.
  2015; 17 (21): 14096-14106
- **Discovering chemistry with an ab initio nanoreactor** *NATURE CHEMISTRY*
  Wang, L., Titov, A., McGibbon, R., Liu, F., Pande, V. S., Martinez, T. J.
  2014; 6 (12): 1044-1048
- **Discovering chemistry with an ab initio nanoreactor (vol 6, pg 1044, 2014)** *NATURE CHEMISTRY*
  Wang, L., Titov, A., McGibbon, R., Liu, F., Pande, V. S., Martinez, T. J.
  2014; 6 (12)
- **Interfacing the Ab Initio Multiple Spawning Method with Electronic Structure Methods in GAMESS: Photodecay of trans-Azonnethane** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Gaenko, A., DeFusco, A., Varganov, S. A., Martinez, T. J., Gordon, M. S.
  2014; 118 (46): 10902-10908
- **A remote stereochemical lever arm effect in polymer mechanochemistry.** *Journal of the American Chemical Society*
  Wang, J., Kouznetsova, T. B., Kean, Z. S., Fan, L., Mar, B. D., Martínez, T. J., Craig, S. L.
  2014; 136 (43): 15162-15165
- **Ab initio nonadiabatic dynamics of multichromophore complexes: a scalable graphical-processing-unit-accelerated exciton framework.** *Accounts of chemical research*
  Sisto, A., Glowacki, D. R., Martinez, T. J.
  2014; 47 (9): 2857-66
- **Ab Initio Nonadiabatic Dynamics of Multichromophore Complexes: A Scalable Graphical-Processing-Unit-Accelerated Exciton Framework** *ACCOUNTS OF CHEMICAL RESEARCH*
  Sisto, A., Glowacki, D. R., Martinez, T. J.
  2014; 47 (9): 2857-2866
- **Direct QM/MM simulation of photoexcitation dynamics in bacteriorhodopsin and halorhodopsin** *CHEMICAL PHYSICS LETTERS*
  Punwong, C., Martinez, T. J., HANNONGBUA, S.
  2014; 610: 213-218
- **Theoretical insight on mechanical sensitivity of chemical reactions rates from ab initio molecular dynamics free energy modeling**
  Plotnikov, N. V., Martinez, T. J.
  AMER CHEMICAL SOC.2014
- **Reduced scaling in electronic structure theory via tensor hypercontraction**
  Hohenstein, E. G., Parrish, R. M., Martinez, T. J.
  AMER CHEMICAL SOC.2014
- **Building force fields: An automatic, systematic and reproducible approach**
  Wang, L., Martinez, T. J., Pande, V. S.
  AMER CHEMICAL SOC.2014
- **Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics.** *journal of chemical physics*
  Makhov, D. V., Glover, W. J., Martinez, T. J., Shalashilin, D. V.
  2014; 141 (5): 054110-?
- **Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer** *NATURE CHEMISTRY*
  Diesendruck, C. E., Peterson, G. I., Kulik, H. J., Kaitz, J. A., Mar, B. D., May, P. A., White, S. R., Martinez, T. J., Boydston, A. J., Moore, J. S.
  2014; 6 (7): 624-629
- **Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations.** *Physical chemistry chemical physics*
  Wolf, T. J., Kuhlman, T. S., Schalk, O., Martínez, T. J., Møller, K. B., Stolow, A., Unterreiner, A.
  2014; 16 (23): 11770-11779

- **Steric and electrostatic effects on photoisomerization dynamics using QM/MM ab initio multiple spawning** *THEORETICAL CHEMISTRY ACCOUNTS*
  Virshup, A. M., Levine, B. G., Martinez, T. J.
  2014; 133 (7)
- **Building Force Fields: An Automatic, Systematic, and Reproducible Approach** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Wang, L., Martinez, T. J., Pande, V. S.
  2014; 5 (11): 1885-1891
- **Ultrafast X-ray Auger probing of photoexcited molecular dynamics** *NATURE COMMUNICATIONS*
  McFarland, B. K., Farrell, J. P., Miyabe, S., Tarantelli, F., Aguilar, A., Berrah, N., Bostedt, C., Bozek, J. D., Bucksbaum, P. H., Castagna, J. C., Coffee, R. N., Cryan, J. P., Fang, et al
  2014; 5
- **Steric and electronic contributions to the core reactivity of monoprotonated 5-phenylporphyrin: A DFT study** *CHEMICAL PHYSICS LETTERS*
  Presselt, M., Wojdyr, M., Beenken, W. J., Kruk, M., Martinez, T. J.
  2014; 603: 21-27
- **Communication: Acceleration of coupled cluster singles and doubles via orbital-weighted least-squares tensor hypercontraction.** *journal of chemical physics*
  Parrish, R. M., Sherrill, C. D., Hohenstein, E. G., Kokkila, S. I., Martínez, T. J.
  2014; 140 (18): 181102-?
- **Photochemical Dynamics of Ethylene Cation C2H4+** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Joalland, B., Mori, T., Martinez, T. J., Suits, A. G.
  2014; 5 (8): 1467-1471
- **Multiple time step integrators in ab initio molecular dynamics.** *journal of chemical physics*
  Luehr, N., Markland, T. E., Martínez, T. J.
  2014; 140 (8): 084116-?
- **Axis-dependence of molecular high harmonic emission in three dimensions.** *Nature communications*
  Spector, L. S., Artamonov, M., Miyabe, S., Martinez, T., Seideman, T., Guehr, M., Bucksbaum, P. H.
  2014; 5: 3190-?
- **Modeling mechanophore activation within a viscous rubbery network** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
  Silberstein, M. N., Cremar, L. D., Beiermann, B. A., Kramer, S. B., Martinez, T. J., White, S. R., Sottos, N. R.
  2014; 63: 141-153
- **Systematic Improvement on the Classical Molecular Model of Water**
  Wang, L., Head-Gordon, T., Ponder, J., Ren, P., Chodera, J., Eastman, P., Martinez, T. J., Pande, V. S.
  CELL PRESS.2014: 403A
- **Ultrafast X-ray Auger probing of photoexcited molecular dynamics.** *Nature communications*
  McFarland, B. K., Farrell, J. P., Miyabe, S., Tarantelli, F., Aguilar, A., Berrah, N., Bostedt, C., Bozek, J. D., Bucksbaum, P. H., Castagna, J. C., Coffee, R. N., Cryan, J. P., Fang, et al
  2014; 5: 4235-?
- **Enhancement of strong-field multiple ionization in the vicinity of the conical intersection in 1,3-cyclohexadiene ring opening** *JOURNAL OF CHEMICAL PHYSICS*
  Petrovic, V. S., Schorb, S., Kim, J., White, J., Cryan, J. P., Glownia, J. M., Zipp, L., Broege, D., Miyabe, S., Tao, H., Martinez, T., Bucksbaum, P. H.
  2013; 139 (18)
- **Tensor Hypercontraction Equation-of-Motion Second-Order Approximate Coupled Cluster: Electronic Excitation Energies in O(N-4) Time** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Hohenstein, E. G., Kokkila, S. I., Parrish, R. M., Martinez, T. J.
  2013; 117 (42): 12972-12978
- **The Charge Transfer Problem in Density Functional Theory Calculations of Aqueously Solvated Molecules** *JOURNAL OF PHYSICAL CHEMISTRY B*

Isborn, C. M., Mar, B. D., Curchod, B. F., Tavernelli, I., Martinez, T. J.
2013; 117 (40): 12189-12201

- **Exact Tensor Hypercontraction: A Universal Technique for the Resolution of Matrix Elements of Local Finite-Range N-Body Potentials in Many-Body Quantum Problems** *PHYSICAL REVIEW LETTERS*
  Parrish, R. M., Hohenstein, E. G., Schunck, N. F., Sherrill, C. D., Martinez, T. J.
  2013; 111 (13)
- **Photochemical dynamics on excited states in ethylene cation**
  Joalland, B. Y., Mori, T., Martinez, T. J., Suits, A. G.
  AMER CHEMICAL SOC.2013
- **Tensor hypercontraction and graphical processing units for electronic structure and ab initio molecular dynamics**
  Martinez, T. J., Hohenstein, E., Kokkila, S. I. L., Ufimtsev, I. S., Luehr, N., Parrish, R.
  AMER CHEMICAL SOC.2013
- **Enhanced strong-field multiple ionization in the vicinity of S-1/S-0 conical intersection in 1,3-cyclohexadiene**
  Petrovic, V., Schorb, S., Kim, J., White, J., Cryan, J., Glownia, J. M., Zipp, L., Broege, D., Miyabe, S., Tao, H., Martinez, T., Bucksbaum, P.
  AMER CHEMICAL SOC.2013
- **ForceBalance, a method for developing better force fields**
  Wang, L., Van Voorhis, T., Martinez, T. J., Pande, V. S.
  AMER CHEMICAL SOC.2013
- **Systematic improvement on the classical molecular model of water**
  Wang, L., Head-Gordon, T., Ponder, J. W., Ren, P., Chodera, J. D., Eastman, P. K., Martinez, T. J., Pande, V. S.
  AMER CHEMICAL SOC.2013
- **Interactive ab initio molecular dynamics**
  Luehr, N., Jin, A., Martinez, T. J.
  AMER CHEMICAL SOC.2013
- **Rotational dynamics of water near protein binding sites: Insights from ab initio molecular dynamics simulation**
  Ufimtsev, I. S., Martinez, T. J.
  AMER CHEMICAL SOC.2013
- **Systematic improvement of a classical molecular model of water.** *journal of physical chemistry. B*
  Wang, L., Head-Gordon, T., Ponder, J. W., Ren, P., Chodera, J. D., Eastman, P. K., Martinez, T. J., Pande, V. S.
  2013; 117 (34): 9956-9972
- **Relation of exact Gaussian basis methods to the dephasing representation: Theory and application to time-resolved electronic spectra** *JOURNAL OF CHEMICAL PHYSICS*
  Sulc, M., Hernandez, H., Martinez, T. J., Vanicek, J.
  2013; 139 (3)
- **Modeling mechanophore activation within a crosslinked glassy matrix** *JOURNAL OF APPLIED PHYSICS*
  Silberstein, M. N., Min, K., Cremar, L. D., Degen, C. M., Martinez, T. J., Aluru, N. R., White, S. R., Sottos, N. R.
  2013; 114 (2)
- **Discrete variable representation in electronic structure theory: Quadrature grids for least-squares tensor hypercontraction** *JOURNAL OF CHEMICAL PHYSICS*
  Parrish, R. M., Hohenstein, E. G., Martinez, T. J., Sherrill, C. D.
  2013; 138 (19)
- **Time resolved photoelectron spectroscopy from first principles nonadiabatic dynamics**
  Martinez, T. J.
  AMER CHEMICAL SOC.2013
- **Quartic scaling second-order approximate coupled cluster singles and doubles via tensor hypercontraction: THC-CC2** *JOURNAL OF CHEMICAL PHYSICS*
  Hohenstein, E. G., Kokkila, S. I., Parrish, R. M., Martinez, T. J.

2013; 138 (12)

- **Exploring the Conical Intersection Seam: The Seam Space Nudged Elastic Band Method.** *Journal of chemical theory and computation*
  Mori, T., Martínez, T. J.
  2013; 9 (2): 1155-63
- **Exploring the Conical Intersection Seam: The Seam Space Nudged Elastic Band Method** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Mori, T., Martinez, T. J.
  2013; 9 (2): 1155-1163
- **Generating Efficient Quantum Chemistry Codes for Novel Architectures.** *Journal of chemical theory and computation*
  Titov, A. V., Ufimtsev, I. S., Luehr, N., Martinez, T. J.
  2013; 9 (1): 213-21
- **Generating Efficient Quantum Chemistry Codes for Novel Architectures** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Titov, A. V., Ufimtsev, I. S., Luehr, N., Martinez, T. J.
  2013; 9 (1): 213-221
- **Probing nucleobase photoprotection with soft x-rays** *18th International Conference on Ultrafast Phenomena*
  McFarland, B. K., Farrell, J. P., Berrah, N., Bostedt, C., Bozek, J., Bucksbaum, P. H., Coffee, R., Cryan, J., Fang, L., Feifel, R., Gaffney, K., Glownia, J., Martinez, et al
  E D P SCIENCES.2013
- **Communication: Tensor hypercontraction. III. Least-squares tensor hypercontraction for the determination of correlated wavefunctions** *JOURNAL OF CHEMICAL PHYSICS*
  Hohenstein, E. G., Parrish, R. M., Sherrill, C. D., Martinez, T. J.
  2012; 137 (22)
- **Nonlinear dimensionality reduction for nonadiabatic dynamics: The influence of conical intersection topography on population transfer rates** *JOURNAL OF CHEMICAL PHYSICS*
  Virshup, A. M., Chen, J., Martinez, T. J.
  2012; 137 (22)
- **Tensor hypercontraction. II. Least-squares renormalization** *JOURNAL OF CHEMICAL PHYSICS*
  Parrish, R. M., Hohenstein, E. G., Martinez, T. J., Sherrill, C. D.
  2012; 137 (22)
- **Electronic Absorption Spectra from MM and ab Initio QM/MM Molecular Dynamics: Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Isborn, C. M., Goetz, A. W., Clark, M. A., Walker, R. C., Martinez, T. J.
  2012; 8 (12): 5092-5106
- **Electronic Absorption Spectra from MM and ab initio QM/MM Molecular Dynamics: Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein.** *Journal of chemical theory and computation*
  Isborn, C. M., Götz, A. W., Clark, M. A., Walker, R. C., Martínez, T. J.
  2012; 8 (12): 5092-5106
- **Ab Initio Quantum Chemistry for Protein Structures** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Kulik, H. J., Luehr, N., Ufimtsev, I. S., Martinez, T. J.
  2012; 116 (41): 12501-12509
- **Charge-transfer states in the nonadiabatic dynamics of photoexcited trans-butadiene**
  Glover, W. J., Martinez, T. J.
  AMER CHEMICAL SOC.2012
- **Predictive enzyme catalysis and protein structure with quantum chemistry on the GPU**
  Kulik, H. J., Martinez, T. J.
  AMER CHEMICAL SOC.2012
- **Ab initio QM/MM molecular dynamics using TeraChem and AMBER: Exploring environmental effects on the absorption spectrum of photoactive yellow protein**

Isborn, C. M., Goetz, A. W., Clark, M., Martinez, T. J., Walker, R. C.
AMER CHEMICAL SOC.2012

- **Photodynamics and spectroscopy in chemical and biological systems: The full multiple spawning method with thermal statistics**
  Liu, J., Martinez, T.
  AMER CHEMICAL SOC.2012
- **Excitation and charge transport with first principles dynamics**
  Martinez, T. J.
  AMER CHEMICAL SOC.2012
- **Tensor hypercontraction density fitting. I. Quartic scaling second- and third-order Moller-Plesset perturbation theory** *JOURNAL OF CHEMICAL PHYSICS*
  Hohenstein, E. G., Parrish, R. M., Martinez, T. J.
  2012; 137 (4)
- **Transient X-Ray Fragmentation: Probing a Prototypical Photoinduced Ring Opening** *PHYSICAL REVIEW LETTERS*
  Petrovic, V. S., Siano, M., White, J. L., Berrah, N., Bostedt, C., Bozek, J. D., Broege, D., Chalfin, M., Coffee, R. N., Cryan, J., Fang, L., Farrell, J. P., Frasinski, et al
  2012; 108 (25)
- **Ultrafast internal conversion in ethylene. II. Mechanisms and pathways for quenching and hydrogen elimination** *JOURNAL OF CHEMICAL PHYSICS*
  Allison, T. K., Tao, H., Glover, W. J., Wright, T. W., Stooke, A. M., Khurmi, C., van Tilborg, J., Liu, Y., Falcone, R. W., Martinez, T. J., Belkacem, A.
  2012; 136 (12)
- **Converging to the basis set limit using empirical correction potentials**
  Wang, L., Martinez, T., Pande, V.
  AMER CHEMICAL SOC.2012
- **Markov-state model analysis of systems containing identical and exchangable components using an optimally permuted RMSD metric**
  Wang, L., Pande, V., Martinez, T.
  AMER CHEMICAL SOC.2012
- **Role of Rydberg States in the Photochemical Dynamics of Ethylene** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Mori, T., Glover, W. J., Schuurman, M. S., Martinez, T. J.
  2012; 116 (11): 2808-2818
- **Control of 1,3-Cyclohexadiene Photoisomerization Using Light-Induced Conical Intersections** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Kim, J., Tao, H., White, J. L., Petrovic, V. S., Martinez, T. J., Bucksbaum, P. H.
  2012; 116 (11): 2758-2763
- **Between ethylene and polyenes - the non-adiabatic dynamics of cis-dienes** *FARADAY DISCUSSIONS*
  Kuhlman, T. S., Glover, W. J., Mori, T., Moller, K. B., Martinez, T. J.
  2012; 157: 193-212
- **Ultrafast X-ray probe of Nucleobase Photoprotection** *Conference on Lasers and Electro-Optics (CLEO)*
  Farrell, J. P., McFarland, B. K., Berrah, N., Bostedt, C., Bozek, J., Bucksbaum, P. H., Coffee, R., Cryan, J., Fang, L., Feifel, R., Gaffney, K., Glownia, J., Martinez, et al
  IEEE.2012
- **A scheme to interpolate potential energy surfaces and derivative coupling vectors without performing a global diabatization** *JOURNAL OF CHEMICAL PHYSICS*
  Evenhuis, C., Martinez, T. J.
  2011; 135 (22)
- **Charge Transfer and Polarization in Solvated Proteins from Ab Initio Molecular Dynamics** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Ufimtsev, I. S., Luehr, N., Martinez, T. J.
  2011; 2 (14): 1789-1793
- **Ultrafast internal conversion in ethylene. I. The excited state lifetime** *JOURNAL OF CHEMICAL PHYSICS*

Tao, H., Allison, T. K., Wright, T. W., Stooke, A. M., Khurmi, C., van Tilborg, J., Liu, Y., Falcone, R. W., Belkacem, A., Martinez, T. J.
2011; 134 (24)

- **Excited-State Electronic Structure with Configuration Interaction Singles and Tamm-Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Isborn, C. M., Luehr, N., Ufimtsev, I. S., Martinez, T. J.
  2011; 7 (6): 1814-1823
- **Dynamic Precision for Electron Repulsion Integral Evaluation on Graphical Processing Units (GPUs).** *Journal of chemical theory and computation*
  Luehr, N., Ufimtsev, I. S., Martínez, T. J.
  2011; 7 (4): 949-54
- **Dynamic Precision for Electron Repulsion Integral Evaluation on Graphical Processing Units (GPUs)** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Luehr, N., Ufimtsev, I. S., Martinez, T. J.
  2011; 7 (4): 949-954
- **Reactive Cross-Talk between Adjacent Tension-Trapped Transition States** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Lenhardt, J. M., Ogle, J. W., Ong, M. T., Choe, R., Martinez, T. J., Craig, S. L.
  2011; 133 (10): 3222-3225
- **Conformationally selective photodissociation dynamics of propanal cation** *JOURNAL OF CHEMICAL PHYSICS*
  Tao, H., Shen, L., Kim, M. H., Suits, A. G., Martinez, T. J.
  2011; 134 (5)
- **Time-resolved photoelectron spectroscopy from first principles: Excited state dynamics of benzene** *FARADAY DISCUSSIONS*
  Thompson, A. L., Martinez, T. J.
  2011; 150: 293-311
- **PHYSICAL CHEMISTRY Seaming is believing** *NATURE*
  Martinez, T. J.
  2010; 467 (7314): 412-413
- **Trapping a Diradical Transition State by Mechanochemical Polymer Extension** *SCIENCE*
  Lenhardt, J. M., Ong, M. T., Choe, R., Evenhuis, C. R., Martinez, T. J., Craig, S. L.
  2010; 329 (5995): 1057-1060
- **Calculating molecular integrals of d and higher angular momentum functions on GPUs**
  Titov, A. V., Ufimtsev, I., Martinez, T., Dunning, T. H.
  AMER CHEMICAL SOC.2010
- **High-Performance Computing with Accelerators INTRODUCTION** *COMPUTING IN SCIENCE & ENGINEERING*
  Kindratenko, V., Wilhelmson, R., Brunner, R., Martinez, T. J., Hwu, W.
  2010; 12 (4): 12-16
- **Ab initio floating occupation molecular orbital-complete active space configuration interaction: An efficient approximation to CASSCF** *JOURNAL OF CHEMICAL PHYSICS*
  Slavicek, P., Martinez, T. J.
  2010; 132 (23)
- **Optimization of width parameters for quantum dynamics with frozen Gaussian basis sets** *CHEMICAL PHYSICS*
  Thompson, A. L., Punwong, C., Martinez, T. J.
  2010; 370 (1-3): 70-77
- **Masked Cyanoacrylates Unveiled by Mechanical Force** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Kryger, M. J., Ong, M. T., Odom, S. A., Sottos, N. R., White, S. R., Martinez, T. J., Moore, J. S.
  2010; 132 (13): 4558-?
- **Variational geminal-augmented multireference self-consistent field theory: Two-electron systems** *JOURNAL OF CHEMICAL PHYSICS*
  Varganov, S. A., Martinez, T. J.

2010; 132 (5)

- **Protonic Gating of Excited-State Twisting and Charge Localization in GFP Chromophores: A Mechanistic Hypothesis for Reversible Photoswitching** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Olsen, S., Lamothe, K., Martinez, T. J.
  2010; 132 (4): 1192-?
- **Ab Initio Multiple Spawning Dynamics Using Multi-State Second-Order Perturbation Theory** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Tao, H., Levine, B. G., Martinez, T. J.
  2009; 113 (49): 13656-13662
- **Ab Initio Multiple Spawning Dynamics of Excited Butadiene: Role of Charge Transfer** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Levine, B. G., Martinez, T. J.
  2009; 113 (46): 12815-12824
- **Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field (SCF) Implementation.** *Journal of chemical theory and computation*
  Ufimtsev, I. S., Martinez, T. J.
  2009; 5 (11): 3138-?
- **Quantum Chemistry on Graphical Processing Units. 3. Analytical Energy Gradients, Geometry Optimization, and First Principles Molecular Dynamics.** *Journal of chemical theory and computation*
  Ufimtsev, I. S., Martinez, T. J.
  2009; 5 (10): 2619-28
- **Quantum Chemistry on Graphical Processing Units. 3. Analytical Energy Gradients, Geometry Optimization, and First Principles Molecular Dynamics** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Ufimtsev, I. S., Martinez, T. J.
  2009; 5 (10): 2619-2628
- **Observation of a Zundel-like transition state during proton transfer in aqueous hydroxide solutions** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Roberts, S. T., Petersen, P. B., Ramasesha, K., Tokmakoff, A., Ufimtsev, I. S., Martinez, T. J.
  2009; 106 (36): 15154-15159
- **Charge conservation in electronegativity equalization and its implications for the electrostatic properties of fluctuating-charge models** *JOURNAL OF CHEMICAL PHYSICS*
  Chen, J., Martinez, T. J.
  2009; 131 (4)
- **First Principles Dynamics and Minimum Energy Pathways for Mechanochemical Ring Opening of Cyclobutene** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Ong, M. T., Leiding, J., Tao, H., Virshup, A. M., Martinez, T. J.
  2009; 131 (18): 6377-?
- **Force-induced activation of covalent bonds in mechanoresponsive polymeric materials** *NATURE*
  Davis, D. A., Hamilton, A., Yang, J., Cremar, L. D., Van Gough, D., Potisek, S. L., Ong, M. T., Braun, P. V., Martinez, T. J., White, S. R., Moore, J. S., Sottos, N. R.
  2009; 459 (7243): 68-72
- **Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field Implementation.** *Journal of chemical theory and computation*
  Ufimtsev, I. S., Martinez, T. J.
  2009; 5 (4): 1004-15
- **Revisiting Molecular Dissociation in Density Functional Theory: A Simple Model.** *Journal of chemical theory and computation*
  Tempel, D. G., Martínez, T. J., Maitra, N. T.
  2009; 5 (4): 770-80
- **An "optimal" spawning algorithm for adaptive basis set expansion in nonadiabatic dynamics** *JOURNAL OF CHEMICAL PHYSICS*
  Yang, S., Coe, J. D., Kaduk, B., Martinez, T. J.

2009; 130 (13)

- **Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field Implementation** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Ufimtsev, I. S., Martinez, T. J.
  2009; 5 (4): 1004-1015
- **Revisiting Molecular Dissociation in Density Functional Theory: A Simple Model** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Tempel, D. G., Martinez, T. J., Maitra, N. T.
  2009; 5 (4): 770-780
- **Photodynamics in Complex Environments: Ab Initio Multiple Spawning Quantum Mechanical/Molecular Mechanical Dynamics** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Virshup, A. M., Punwong, C., Pogorelov, T. V., Lindquist, B. A., Ko, C., Martinez, T. J.
  2009; 113 (11): 3280-3291
- **Nonclassical Phase Space Jumps and Optimal Spawning** *13th International Workshop on Quantum Systems in Chemistry and Physics*
  Yang, S., Martinez, T. J.
  SPRINGER.2009: 35–45
- **Implementation of scientific computing applications on the Cell Broadband Engine** *SCIENTIFIC PROGRAMMING*
  Shi, G., Kindratenko, V. V., Ufimtsev, I. S., Martinez, T. J., Phillips, J. C., Gottlieb, S. A.
  2009; 17 (1-2): 135-151
- **A multistate empirical valence bond model for solvation and transport simulations of OH- in aqueous solutions** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
  Ufimtsev, I. S., Kalinichev, A. G., Martinez, T. J., Kirkpatrick, R. J.
  2009; 11 (41): 9420-9430
- **The Dissociation Catastrophe in Fluctuating-Charge Models and its Implications for the Concept of Atomic Electronegativity** *13th International Workshop on Quantum Systems in Chemistry and Physics*
  Chen, J., Martinez, T. J.
  SPRINGER.2009: 397–415
- **On the Extent and Connectivity of Conical Intersection Seams and the Effects of Three-State Intersections** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Coe, J. D., Ong, M. T., Levine, B. G., Martinez, T. J.
  2008; 112 (49): 12559-12567
- **A unified theoretical framework for fluctuating-charge models in atom-space and in bond-space** *JOURNAL OF CHEMICAL PHYSICS*
  Chen, J., Hundertmark, D., Martinez, T. J.
  2008; 129 (21)
- **Excited-State Dynamics of Cytosine Reveal Multiple Intrinsic Subpicosecond Pathways** *CHEMPHYSCHEM*
  Hudock, H. R., Martinez, T. J.
  2008; 9 (17): 2486-2490
- **Graphical Processing Units for Quantum Chemistry** *COMPUTING IN SCIENCE & ENGINEERING*
  Ufimtsev, I. S., Martinez, T. J.
  2008; 10 (6): 26-34
- **QTPIE: Charge transfer with polarization current equalization. A fluctuating charge model with correct asymptotics (vol 438, pg 315, 2007)** *CHEMICAL PHYSICS LETTERS*
  Chen, J., Martinez, T. J.
  2008; 463 (1-3): 288-288
- **Electrostatic control of photoisomerization in the photoactive yellow protein chromophore: Ab initio multiple spawning dynamics** *CHEMICAL PHYSICS LETTERS*
  Ko, C., Virshup, A. M., Martinez, T. J.
  2008; 460 (1-3): 272-277

- **Ultrafast photoinduced processes in polyatomic molecules: Electronic structure, dynamics and spectroscopy (in honour of Wolfgang Domcke) - Preface** *CHEMICAL PHYSICS*
  Thoss, M., Stock, G., Martinez, T. J.
  2008; 347 (1-3): 1-2
- **Implementation of ab initio multiple spawning in the MOLPRO quantum chemistry package** *CHEMICAL PHYSICS*
  Levine, B. G., Coe, J. D., Virshup, A. M., Martinez, T. J.
  2008; 347 (1-3): 3-16
- **Pseudospectral time-dependent density functional theory** *JOURNAL OF CHEMICAL PHYSICS*
  Ko, C., Malick, D. K., Braden, D. A., Friesner, R. A., Martinez, T. J.
  2008; 128 (10)
- **Quantum chemistry on graphical processing units. 1. Strategies for two-electron integral evaluation** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Ufimtsev, I. S., Martinez, T. J.
  2008; 4 (2): 222-231
- **Quantum Chemistry on Graphical Processing Units. 1. Strategies for Two-Electron Integral Evaluation.** *Journal of chemical theory and computation*
  Ufimtsev, I. S., Martínez, T. J.
  2008; 4 (2): 222-31
- **Optimizing conical intersections without derivative coupling vectors: Application to multistate multireference second-order perturbation theory (MS-CASPT2)** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Levine, B. G., Coe, J. D., Martinez, T. J.
  2008; 112 (2): 405-413
- **Ab initio multiple spawning dynamics of excited state intramolecular proton transfer: the role of spectroscopically dark states** *MOLECULAR PHYSICS*
  Coe, J. D., Martinez, T. J.
  2008; 106 (2-4): 537-545
- **Substituent effects on dynamics at conical intersections: alpha,beta-enones** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Lee, A. M., Coe, J. D., Ullrich, S., Ho, M., Lee, S., Cheng, B., Zgierski, M. Z., Chen, I., Martinez, T. J., Stolow, A.
  2007; 111 (47): 11948-11960
- **Ab initio molecular dynamics of excited-state intramolecular proton transfer using multireference perturbation theory** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Coe, J. D., Levine, B. G., Martinez, T. J.
  2007; 111 (44): 11302-11310
- **Comparative genomics and site-directed mutagenesis support the existence of only one input channel for protons in the C-family (cbb(3) oxidase) of heme-copper oxygen reductases** *BIOCHEMISTRY*
  Hemp, J., Han, H., Roh, J. H., Kaplan, S., Martinez, T. J., Gennis, R. B.
  2007; 46 (35): 9963-9972
- **Ab initio molecular dynamics and time-resolved photoelectron spectroscopy of electronically excited uracil and thymine** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Hudock, H. R., Levine, B. G., Thompson, A. L., Satzger, H., Townsend, D., Gador, N., Ullrich, S., Stolow, A., Martinez, T. J.
  2007; 111 (34): 8500-8508
- **A charged ring model for classical OH-(aq) simulations** *CHEMICAL PHYSICS LETTERS*
  Ufimtsev, I. S., Kalinichev, A. G., Martinez, T. J., Kirkpatrick, R. J.
  2007; 442 (1-3): 128-133
- **The vibrationally adiabatic torsional potential energy surface of trans-stilbene** *CHEMICAL PHYSICS LETTERS*
  Chowdary, P. D., Martinez, T. J., Gruebele, M.
  2007; 440 (1-3): 7-11

- **QTPIE: Charge transfer with polarization current equalization. A fluctuating charge model with correct asymptotics** *CHEMICAL PHYSICS LETTERS*
  Chen, J., Martinez, T. J.
  2007; 438 (4-6): 315-320
- **Conformationally controlled chemistry: Excited-state dynamics dictate ground-state reaction** *SCIENCE*
  Kim, M. H., Shen, L., Tao, H., Martinez, T. J., Suits, A. G.
  2007; 315 (5818): 1561-1565
- **A continuous spawning method for nonadiabatic dynamics and validation for the zero-temperature spin-boson problem** *ISRAEL JOURNAL OF CHEMISTRY*
  Ben-Nun, M., Martinez, T. J.
  2007; 47 (1): 75-88
- **Optimization of semiempirical quantum chemistry methods via multiobjective genetic algorithms: Accurate photodynamics for larger molecules and longer time scales** *MATERIALS AND MANUFACTURING PROCESSES*
  Sastry, K., Johnson, D. D., Thompson, A. L., Goldberg, D. E., Martinez, T. J., Leiding, J., Owens, J.
  2007; 22 (5-6): 553-561
- **The evolutionary migration of a post-translationally modified active-site residue in the proton-pumping heme-copper oxygen reductases** *51st Annual Meeting of the Biophysical-Society*
  Robinson, D., Hemp, J., Kelleher, N. L., Martinez, T. J., Gennis, R. B.
  CELL PRESS.2007: 502A–502A
- **First principles dynamics of photoexcited DNA and RNA bases** *International Conference on Computational Methods in Science and Engineering*
  Hudock, H. R., Levine, B. G., Thompson, A. L., Martinez, T. J.
  AMER INST PHYSICS.2007: 219–222
- **Isomerization through conical intersections** *ANNUAL REVIEW OF PHYSICAL CHEMISTRY*
  Levine, B. G., Martinez, T. J.
  2007; 58: 613-634
- **Evolutionary migration of a post-translationally modified active-site residue in the proton-pumping heme-copper oxygen reductases** *BIOCHEMISTRY*
  Hemp, J., Robinson, D. E., Ganesan, K. B., Martinez, T. J., Kelleher, N. L., Gennis, R. B.
  2006; 45 (51): 15405-15410
- **Conical intersections and double excitations in time-dependent density functional theory** *MOLECULAR PHYSICS*
  Levine, B. G., Ko, C., Quenneville, J., Martinez, T. J.
  2006; 104 (5-7): 1039-1051
- **Multicentered valence electron effective potentials: A solution to the link atom problem for ground and excited electronic states** *JOURNAL OF CHEMICAL PHYSICS*
  Slavicek, P., Martinez, T. J.
  2006; 124 (8)
- **Insights for light-driven molecular devices from ab initio multiple spawning excited-state dynamics of organic and biological chromophores** *ACCOUNTS OF CHEMICAL RESEARCH*
  Martinez, T. J.
  2006; 39 (2): 119-126
- **Ab initio molecular dynamics of excited-state intramolecular proton transfer around a three-state conical intersection in malonaldehyde** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Coe, J. D., Martinez, T. J.
  2006; 110 (2): 618-630
- **Multiobjective genetic algorithms for multiscaling excited state direct dynamics in photochemistry** *8th Annual Genetic and Evolutionary Computation Conference*
  Sastry, K., Johnson, D. D., Thompson, A. L., Goldberg, D. E., Martinez, T. J., Leiding, J., Owens, J.
  ASSOC COMPUTING MACHINERY.2006: 1745–1752

- **Simulation of the photodynamics of azobenzene on its first excited state: Comparison of full multiple spawning and surface hopping treatments** *JOURNAL OF CHEMICAL PHYSICS*
  Toniolo, A., Ciminelli, C., Persico, M., Martinez, T. J.
  2005; 123 (23)

- **Using meta conjugation to enhance charge separation versus charge recombination in phenylacetylene donor-bridge-acceptor complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Thompson, A. L., Ahn, T. S., Thomas, K. R., Thayumanavan, S., Martinez, T. J., Bardeen, C. J.
  2005; 127 (47): 16348-16349

- **Meta- and para-substitution in aromatic systems: Insights from first-principles dynamics and ultrafast spectroscopy** *230th National Meeting of the American-Chemical-Society*
  Thompson, A. L., Gaab, K. M., Thomas, K. R., Thayumanavan, S., Bardeen, C. J., Martinez, T. J.
  AMER CHEMICAL SOC.2005: U2968–U2969

- **Helix switching of a key active-site residue in the cytochrome cbb(3) oxidases** *BIOCHEMISTRY*
  Hemp, J., Christian, C., Barquera, B., Gennis, R. B., Martinez, T. J.
  2005; 44 (32): 10766-10775

- **Competitive decay at two- and three-state conical intersections in excited-state intramolecular proton transfer** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Coe, J. D., Martinez, T. J.
  2005; 127 (13): 4560-4561

- **Direct QM/MM Simulations of the photodynamics of retinal protonated Schiff base in isolation and solvated environments** *49th Annual Meeting of the Biophysical-Society*
  Punwong, C., Owens, J., Martinez, T. J.
  CELL PRESS.2005: 530A–530A

- **Computation of Reaction Mechanisms and Dynamics in Photobiology** *COMPUTATIONAL PHOTOCHEMISTRY*
  Olsen, S., Toniolo, A., Ko, C., Manohar, L., Lamothe, K., Martinez, T. J.
  edited by Olivucci, M.
  2005; 16: 225-253

- **Ab initio investigation of ionic hydration with the polarizable continuum model** *ASME Heat Transfer Summer Conference*
  Karampinos, D. C., Georgiadis, J. G., Martinez, T. J.
  AMER SOC MECHANICAL ENGINEERS.2005: 473–480

- **Ab initio equation-of-motion coupled-cluster molecular dynamics with 'on-the-fly' diabatization: the doublet-like feature in the photoabsorption spectrum of ethylene** *CHEMICAL PHYSICS LETTERS*
  Choi, H. C., Baeck, K. K., Martinez, T. J.
  2004; 398 (4-6): 407-413

- **Excited state direct dynamics of benzene with reparameterized multi-reference semiempirical configuration interaction methods** *CHEMICAL PHYSICS*
  Toniolo, A., Thompson, A. L., Martinez, T. J.
  2004; 304 (1-2): 133-145

- **Energy and charge transport through conjugated phenylacetylene networks.**
  Bardeen, C. J., Thompson, A. L., Martinez, T., Thayumanavan, S., Thomas, K. R.
  AMER CHEMICAL SOC.2004: U18

- **A new approach to reactive potentials with fluctuating charges: Quadratic valence-bond model** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Morales, J., Martinez, T. J.
  2004; 108 (15): 3076-3084

- **Variable electronic coupling in phenylacetylene dendrimers: The role of forster, dexter, and charge-transfer interactions** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Thompson, A. L., Gaab, K. M., Xu, J. J., Bardeen, C. J., Martinez, T. J.
  2004; 108 (4): 671-682

- **Conical intersection dynamics in solution: the chromophore of Green Fluorescent Protein** *General Meeting on Non-Adiabatic Effects in Chemical Dynamics*
  Toniolo, A., Olsen, S., Manohar, L., Martinez, T. J.
  ROYAL SOC CHEMISTRY.2004: 149–163
- **Helix switching of a key active site residue in the cytochrome cbb(3) oxidases**
  Hemp, J., Martinez, T., Gennis, R.
  BIOPHYSICAL SOCIETY.2004: 305A-306A
- **Azobenzene photoisomerization: Two states and two relaxation pathways explain the violation of Kasha's rule.** *6th International Conference on Femtochemistry*
  Schultz, T., Ullrich, S., Quenneville, J., Martinez, T. J., Zgierski, M. Z., Stolow, A.
  ELSEVIER SCIENCE BV.2004: 45–48
- **Ultrafast excited state dynamics in the green fluorescent protein chromophore** *6th International Conference on Femtochemistry*
  Toniolo, A., Olsen, S., Manohar, L., Martinez, T. J.
  ELSEVIER SCIENCE BV.2004: 425–432
- **Quantum energy flow and trans-stilbene photoisomerization: an example of a non-RRKM reaction** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Leitner, D. M., Levine, B., Quenneville, J., Martinez, T. J., Wolynes, P. G.
  2003; 107 (49): 10706-10716
- **Ab initio excited-state dynamics of the photoactive yellow protein chromophore** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Ko, C., Levine, B., Toniolo, A., Manohar, L., Olsen, S., Werner, H. J., Martinez, T. J.
  2003; 125 (42): 12710-12711
- **Hijacking the playstation2 for computational chemistry.** *226th National Meeting of the American-Chemical-Society*
  Levine, B., Martinez, T. J.
  AMER CHEMICAL SOC.2003: U426–U426
- **Meta-conjugation and excited-state coupling in phenylacetylene dendrimers** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Gaab, K. M., Thompson, A. L., Xu, J. J., Martinez, T. J., Bardeen, C. J.
  2003; 125 (31): 9288-9289
- **Mechanism and dynamics of azobenzene photoisomerization** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Schultz, T., Quenneville, J., Levine, B., Toniolo, A., Martinez, T. J., Lochbrunner, S., Schmitt, M., Shaffer, J. P., Zgierski, M. Z., Stolow, A.
  2003; 125 (27): 8098-8099
- **Ab initio molecular dynamics with equation-of-motion coupled-cluster theory: electronic absorption spectrum of ethylene** *CHEMICAL PHYSICS LETTERS*
  Baeck, K. K., Martinez, T. J.
  2003; 375 (3-4): 299-308
- **The construction of semi-diabatic potential energy surfaces of excited states for use in excited state AIMD studies by the equation-of-motion coupled-cluster method** *10th Korea/Japan Joint Symposium on Theoretical/Computational Chemistry Molecular Structure, Properties, and Design*
  Baeck, K. K., Martinez, T. J.
  KOREAN CHEMICAL SOC.2003: 712–16
- **Electronic structure of solid 1,3,5-triamino-2,4,6-trinitrobenzene under uniaxial compression: Possible role of pressure-induced metallization in energetic materials** *PHYSICAL REVIEW B*
  Wu, C. J., Yang, L. H., Fried, L. E., Quenneville, J., Martinez, T. J.
  2003; 67 (23)
- **Conical intersections in solution: A QM/MM study using floating occupation semiempirical configuration interaction wave functions** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Toniolo, A., Granucci, G., Martinez, T. J.
  2003; 107 (19): 3822-3830
- **Ab initio study of cis-trans photoisomerization in stilbene and ethylene** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Quenneville, J., Martinez, T. J.

2003; 107 (6): 829-837

- **Solvation of the fluoride anion by methanol** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Corbett, C. A., Martinez, T. J., Lisy, J. M.
  2002; 106 (42): 10015-10021
- **Optimization of conical intersections with floating occupation semiempirical configuration interaction wave functions** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Toniolo, A., Ben-Nun, M., Martinez, T. J.
  2002; 106 (18): 4679-4689
- **The role of intersection topography in bond selectivity of cis-trans photoisomerization** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Ben-Nun, M., Molnar, F., Schulten, K., Martinez, T. J.
  2002; 99 (4): 1769-1773
- **Ab initio quantum molecular dynamics** *ADVANCES IN CHEMICAL PHYSICS, VOLUME 121*
  Ben-Nun, M., Martinez, T. J.
  2002; 121: 439-512
- **Features of interest on the S-0 and S-1 potential energy surfaces of a model green fluorescent protein chromophore**
  Olsen, S., Manohar, L., Martinez, T. J.
  CELL PRESS.2002: 359A–359A
- **Photochemistry from first principles - advances and future prospects** *18th IUPAC Symposium on Photochemistry*
  Quenneville, J., Ben-Nun, M., Martinez, T. J.
  ELSEVIER SCIENCE SA.2001: 229–35
- **Comparison of full multiple spawning, trajectory surface hopping, and converged quantum mechanics for electronically nonadiabatic dynamics** *JOURNAL OF CHEMICAL PHYSICS*
  Hack, M. D., Wensmann, A. M., Truhlar, D. G., Ben-Nun, M., Martinez, T. J.
  2001; 115 (3): 1172-1186
- **Classical fluctuating charge theories: The maximum entropy valence bond formalism and relationships to previous models** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Morales, J., Martinez, T. J.
  2001; 105 (12): 2842-2850
- **HYDRA: A program for QM/MM and dynamics calculations**
  Kim, A. J., Olsen, S., Hemp, J., Martinez, T. J.
  CELL PRESS.2001: 322A–322A
- **Photodynamics of ethylene: ab initio studies of conical intersections** *CHEMICAL PHYSICS*
  Ben-Nun, M., Martinez, T. J.
  2000; 259 (2-3): 237-248
- **Characterization of a conical intersection between the ground and first excited state for a retinal analog** *5th World Congress of Theoretically Oriented Chemists (WATOC)*
  Molnar, F., Ben-Nun, M., Martinez, T. J., Schulten, K.
  ELSEVIER SCIENCE BV.2000: 169–178
- **Direct observation of disrotatory ring-opening in photoexcited cyclobutene using ab initio molecular dynamics** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Ben-Nun, M., Martinez, T. J.
  2000; 122 (26): 6299-6300
- **Ab initio multiple spawning: Photochemistry from first principles quantum molecular dynamics** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Ben-Nun, M., Quenneville, J., Martinez, T. J.
  2000; 104 (22): 5161-5175
- **A multiple spawning approach to tunneling dynamics** *JOURNAL OF CHEMICAL PHYSICS*

Ben-Nun, M., Martinez, T. J.
2000; 112 (14): 6113-6121

- **Ab initio study of coupled electron transfer/proton transfer in cytochrome c oxidase** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Moore, D. B., Martinez, T. J.
  2000; 104 (11): 2367-2374
- **Electronic absorption and resonance Raman spectroscopy from ab initio quantum molecular dynamics** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Ben-Nun, M., Martinez, T. J.
  1999; 103 (49): 10517-10527
- **Semiclassical tunneling rates from ab initio molecular dynamics** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Ben-Nun, M., Martinez, T. J.
  1999; 103 (31): 6055-6059
- **The solvation of chloride by methanol - surface versus interior cluster ion states** *JOURNAL OF CHEMICAL PHYSICS*
  Cabarcos, O. M., Weinheimer, C. J., Martinez, T. J., Lisy, J. M.
  1999; 110 (19): 9516-9526
- **Exploiting temporal nonlocality to remove scaling bottlenecks in nonadiabatic quantum dynamics** *JOURNAL OF CHEMICAL PHYSICS*
  Ben-Nun, M., Martinez, T. J.
  1999; 110 (9): 4134-4140
- **Ab initio interpolated quantum dynamics on coupled electronic states with full configuration interaction wave functions** *JOURNAL OF CHEMICAL PHYSICS*
  Thompson, K., Martinez, T. J.
  1999; 110 (3): 1376-1382
- **Ab initio molecular dynamics study of cis-trans photoisomerization in ethylene** *CHEMICAL PHYSICS LETTERS*
  Ben-Nun, M., Martinez, T. J.
  1998; 298 (1-3): 57-65
- **Electronic energy funnels in cis-trans photoisomerization of retinal protonated Schiff base** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Ben-Nun, M., Martinez, T. J.
  1998; 102 (47): 9607-9617
- **Direct evaluation of the Pauli repulsion energy using 'classical' wavefunctions in hybrid quantum/classical potential energy surfaces** *CHEMICAL PHYSICS LETTERS*
  Ben-Nun, M., Martinez, T. J.
  1998; 290 (1-3): 289-295
- **Nonadiabatic molecular dynamics: Validation of the multiple spawning method for a multidimensional problem** *JOURNAL OF CHEMICAL PHYSICS*
  Ben-Nun, M., Martinez, T. J.
  1998; 108 (17): 7244-7257
- **Quantum dynamics of the femtosecond photoisomerization of retinal in bacteriorhodopsin** *FARADAY DISCUSSIONS*
  Ben-Nun, M., Molnar, F., Lu, H., Phillips, J. C., Martinez, T. J., Schulten, K.
  1998; 110: 447-462
- **Nonstationary electronic states and site-selective reactivity** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Weinkauf, R., Schlag, E. W., Martinez, T. J., Levine, R. D.
  1997; 101 (42): 7702-7710
- **Dynamical stereochemistry on several electronic states: A computational study of Na*+H-2** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Bennun, M., Martinez, T. J., Levine, R. D.
  1997; 101 (41): 7522-7529
- **Molecular collision dynamics on several electronic states** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Martinez, T. J., Bennun, M., Levine, R. D.

1997; 101 (36): 6389-6402

- **Ab initio molecular dynamics around a conical intersection: Li(2p)+H-2** *CHEMICAL PHYSICS LETTERS*
  Martinez, T. J.
  1997; 272 (3-4): 139-147
- **Multiple traversals of a conical intersection: electronic quenching in Na*+H-2** *CHEMICAL PHYSICS LETTERS*
  Bennun, M., Martinez, T. J., Levine, R. D.
  1997; 270 (3-4): 319-326
- **Non-adiabatic molecular dynamics: Split-operator multiple spawning with applications to photodissociation** *JOURNAL OF THE CHEMICAL SOCIETY-FARADAY TRANSACTIONS*
  Martinez, T. J., Levine, R. D.
  1997; 93 (5): 941-947
- **Direct imaging of excited electronic states using diffraction techniques: Theoretical considerations** *CHEMICAL PHYSICS LETTERS*
  Bennun, M., Martinez, T. J., Weber, P. M., Wilson, K. R.
  1996; 262 (3-4): 405-414
- **First-principles molecular dynamics on multiple electronic states: A case study of NaI** *JOURNAL OF CHEMICAL PHYSICS*
  Martinez, T. J., Levine, R. D.
  1996; 105 (15): 6334-6341
- **Dynamics of the collisional electron transfer and femtosecond photodissociation of NaI on ab initio electronic energy curves** *CHEMICAL PHYSICS LETTERS*
  Martinez, T. J., Levine, R. D.
  1996; 259 (3-4): 252-260
- **Multi-electronic-state molecular dynamics: A wave function approach with applications** *JOURNAL OF PHYSICAL CHEMISTRY*
  Martinez, T. J., Bennun, M., Levine, R. D.
  1996; 100 (19): 7884-7895
- **Classical quantal method for multistate dynamics: A computational study** *JOURNAL OF CHEMICAL PHYSICS*
  Martinez, T. J., Bennun, M., Ashkenazi, G.
  1996; 104 (8): 2847-2856

PRESENTATIONS

- Q & A with Todd Martínez: GPU-Accelerated Quantum Chemistry - NVIDIA (January 30, 2014)
- Research news: Stanford chemists develop 'nanoreactor' for discovering new chemical reactions - Stanford News Service (November 17, 2014)
- Lecture, Theoretical & Computation Biophysics Group Summer School 2003: Quantum Chemistry of Proteins - Introduction and Examples - Theoretical & Computation Biophysics Group Summer School (June 6, 2003)