Stanford

Todd Martinez

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

CONTACT INFORMATION

- **Administrative Contact**

  Maggie Yeung - Administrative Associate

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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 co-editor of Annual Reviews in Physical Chemistry, associate editor of The Journal of Chemical Physics, and an elected fellow of 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

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

- Elected Member, International Academy of Quantum Molecular Sciences (2017)
- Fellow, American Academy of Arts and Sciences (2011)
- National Security Science and Engineering Faculty Fellow, Department of Defense (2010)
- 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)
- Teacher-Scholar Award, Camille & Henry Dreyfus Foundation (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)
- 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)
- Beckman Fellow, UIUC Center for Advanced Study (2000)

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

Teaching

COURSES

2019-20

- Physical Chemistry II: CHEM 173 (Aut)

2018-19

- Physical Chemistry II: CHEM 173 (Aut)

2017-18

- Physical Chemistry II: CHEM 173 (Aut)

2016-17

- Physical Chemistry II: CHEM 173 (Aut)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Michael Angell, Evan Antoniuk, Christian Chamberlayne, Tao Large, Chi-Yun Lin, Tianyi Liu, Sarah Sandholtz

Postdoctoral Faculty Sponsor

Christoph Bannwarth, Roman Ellerbrock, Bryan Fales, Ruibin Liang, Nanna Holmgaard List, Jan Meisner, Elisa Pieri, Umberto Raucci, Elliot Taffet, Alessio Valentini, Alice Walker

Doctoral Dissertation Advisor (AC)

Ethan Curtis, Jason Ford, Soren Holm, Grace Johnson, Chey Jones, David Sanchez, Stefan Seritan, Henry Wang, Hayley Weir, Monika Williams, Jimmy Yu

Doctoral Dissertation Co-Advisor (AC)

Kallie Hilsabeck

Publications

PUBLICATIONS

- **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

- **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
- **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. 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., 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
- **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., 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., Liu, E., Martinez, T. J., Neumark, D. M.
  2019
- **Nonadiabatic Photodynamics of Retinal Protonated Schiff Base in Channelrhodopsin 2.** *The journal of physical chemistry letters*
  Liang, R., Liu, F., 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., Gühr, M.
  2019
- **Perturbation of Short Hydrogen Bonds in Photoactive Yellow Protein via Noncanonical Amino Acid Incorporation.** *The journal of physical chemistry. B*
  Thomson, B., Both, J., Wu, Y., Parrish, R. M., Martínez, T. J., Boxer, S. G.
  2019
- **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
- **Rank reduced coupled cluster theory. I. Ground state energies and wavefunctions.** *The Journal of chemical physics*
  Parrish, R. M., Zhao, Y., Hohenstein, E. G., Martínez, T. J.
  2019; 150 (16): 164118
- **Ab lnitio 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
- **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. 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

- **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

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

- **Ultrafast isomerization in acetylene dication after carbon K-shell ionization** *NATURE COMMUNICATIONS*
  Li, Z., Inhester, L., Liekhus-Schmaltz, C., Curchod, B. 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

- **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

- **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
- **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.
  2017; 147 (16): 164105
- **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): 475–79
- **Description of ground and excited electronic states by ensemble density functional method with extended active space.** *The Journal of chemical physics*
  Filatov, M., 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., 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., Herrmann-Westendorf, F., Ngo, T. H., Martínez, T., Dietzek, B., Hill, J. P., Ariga, K., Kruk, M. M., Maes, W., Presselt, M.
  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

- **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)

- **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., Martinez, 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. P., Martínez, T. J.
  2016; 12 (1): 92–106
- **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 lnitio 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)
- **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.
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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)
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