Stanford

Todd Martinez

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

CONTACT INFORMATION

- **Administrative Contact**

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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
- Member, 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

- Elected Member, National Academy of Sciences (2019)
- 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

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

2023-24

- Chemical Principles I: CHEM 31A (Aut)

2022-23

- Chemical Principles I: CHEM 31A (Aut)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Alex Hart, Matias Horst, Tao Large, Junkun Pan, Nick Werby

Postdoctoral Faculty Sponsor

Melisa Alkan, Dip Hait, Lixin Lu, Johan Nordstrand, Amiel Stephen Paz, Bhaskar Rana, Martin Stoehr, Pablo Unzueta, Rui Xu

Doctoral Dissertation Advisor (AC)

Alex Chang, Ethan Curtis, Jan Estrada Pabon, Otto Fajen, Colton Hicks, Soren Holm, Garrett Kukier, Dean Lahana, Henry Wang, Ruiyan Wang, Laura Weiler, Nancy Zhu

Publications

PUBLICATIONS

- **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 #-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. 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.
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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)
- Lecture, Theoretical & Computation Biophysics Group Summer School 2003: Quantum Chemistry of Proteins - Introduction and Examples - Theoretical & Computation Biophysics Group Summer School (June 6, 2003)