TODD J. MARTINEZ

Department of Chemistry
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Todd.Martinez@stanford.edu

PERSONAL Born March 22, 1968

EDUCATION

Postdoctoral Scholar, University of California, Los Angeles and Hebrew University, Jerusalem, Israel Postdoctoral Advisor: Raphael D. Levine	1994-1996
PhD in Physical Chemistry, University of California, Los Angeles Doctoral Advisor: Emily A. Carter Dissertation topic: *Pseudospectral Treatments of Electron Correlation*	1994
BS in Chemistry, Calvin College, Grand Rapids, MI	1989

ACADEMIC APPOINTMENTS

D. M. Ehrsam and E. C. Franklin Professor, Stanford University	2009-present
Professor of Photon Science, SLAC National Accelerator Laboratory	2009-present
Professor of Chemistry, Stanford University	2009-present
Edward William and Jane Marr Gutgsell Chair in Chemistry, UIUC	2006-2008
Visiting Professor, Ecole Normal Superieure, Paris, France	2006
Professor of Chemistry, UIUC	2004-2009
Associate Professor of Chemistry, UIUC	2002-2004
Faculty Member, UIUC Center for Biophysics and Computational Biology	2000-2008
Affiliate, Beckman Institute for Advanced Science and Technology	1996-2008
Assistant Professor of Chemistry, UIUC	1996-2002

HONORS AND AWARDS

Elected Member, International Academy of Quantum Molecular Science	2017
Elected Fellow, American Academy of Arts and Sciences	2011
National Security Science and Engineering Faculty Fellow (NSSEFF)	2010
Distinguished Alumnus, Carol Morgan School, Dominican Republic	2008
AAAS Fellow, American Association for the Advancement of Science	2006
APS Fellow, American Physical Society	2005
MacArthur Fellow, John D. and Catherine T. MacArthur Foundation	2005
UIUC Excellent Teacher	2005
NSF Special Creativity Extension	2004
UIUC University Scholar	2004
Helen Corley Petit Professor, UIUC College of Liberal Arts and Sciences	2002
UIUC School of Chemical Sciences Excellence in Teaching Award	2001
Teacher Scholar Award, Camille and Henry Dreyfus Foundation	2000
Beckman Fellow, UIUC Center for Advanced Study	2000
Packard Fellow, David and Lucille Packard Foundation	1999
Beckman Young Investigator, Beckman Foundation	1999
Sloan Fellow, Sloan Foundation	1999
Research Innovation Award, Research Corporation	1998
NSF CAREER Award	1998
President's Postdoctoral Fellow, University of California	1994

Fulbright Postdoctoral Fellow	1995
UCLA Excellence in Research Award	1992
NSF Minority Graduate Assistantship	1991
Patricia Harris Roberts Graduate Fellowship	1989

GRANTS RECEIVED (SINCE 2012)

Except for the MRI, only funds allocated to Martínez research are shown (including indirect costs).

National Science Foundation, 2016-2019 $450,000
Tensor Hypercontraction for Electronic Structure and First Principles Molecular Dynamics

Global Climate and Energy Project, 2015-2018 $330,000
Carbonate-Catalyzed CO_2 Hydrogenation to Multi-Carbon Products
(w/M. Kanan)

National Science Foundation, 2015-2016 $112,500
STTR Phase I: An intuitive and tactile quantum mechanical molecular modeling tool for instruction of chemistry students
(w/J. Quenneville, Spectral Sciences)

National Science Foundation, 2015-2019 $600,000
Removing Bottlenecks in High Performance Computational Science
(w/M. Gordon, T. Windus, L. Slipchenko and T. D. Crawford)

National Science Foundation, 2014-2017 $3,500,000
MRI: Acquisition of an Extreme GPU Cluster for Interdisciplinary Research
(w/V. Pande, M. Gerritsen, and T. Abel – this grant funds a computing resource that will be used by both Stanford and national users)

Office of Naval Research /AFOSR, 2014-2017 $850,000
Uncovering Complex Reaction Networks from First Principles

Office of Naval Research, 2012-2017 $1,000,000
Shock Wave Energy Dissipation
(w/D. Dlott, K. Suslick, J. Moore, N. Sottos, A. Strachan)

Department of Energy, 2012-2015 $1,496,520
Ultrafast Theory and Simulation

Department of Energy, 2012-2015 $500,000
Predictive Theory of Transition Metal Oxide Catalysts
(w/J. Norskov, T. Deveraux, C. Campbell, A. Nilsson)

Army Research Office, 2012-2013 $200,000
Mechanically Trapping Transition States and Reactive Intermediates
(w/S. Craig, S. Sheiko)

GRADUATE STUDENTS SUPERVISED

2015-	Jimmy Yu	
2015-	Laszlo Seress	
2015-	David Sanchez	
2015-	Jason Ford	
2015-	Stefan Seritan	
2013-2016	Lin Fan	(MS, 2016)
2013-2015	Nicholas Settje	(MS, 2015)
2012-	James Snyder	
2012-	Chenchen Song	
2011-2016	Aaron Sisto	(PhD, 2016; In-Q-Tel, VA)

2011-2013	Brendan Mar	(MS, 2013)
2011-2016	Sara Kokkila	(PhD, 2016; Postdoctoral, IBM Research)
2011-	Fang Liu	
2011-	Sofia Izmailov	
2010-2014	Nicholas Ward	(PhD, 2016)
2010-2015	Nathan Luehr	(PhD, 2015; Nvidia Corp., CA)
2007-2011	Ivan Ufimtsev	(PhD, 2011; Postdoctoral, Stanford)
2007-2012	Lee Cremar	(PhD, 2012; Postdoctoral, UT Pan Am)
2006-2011	Hongli Tao	(PhD, 2011; Lattice Engines, CA)
2005-2009	Jiahao Chen	(PhD, 2009; Research Scientist, MIT)
2005-2010	Mitchell Ong	(PhD, 2010; Postdoctoral, Livermore National Lab)
2005-2009	Aaron Virshup	(PhD, 2009; Autodesk, CA)
2004-2006	Kristina Lamothe	(MS Biophysics, 2006)
2004-2008	Hanelli Hudock	(PhD, 2008; McKinsey and Co, MA)
2003-2009	Chutintorn Punwong	(PhD, 2009; Asst Prof, Prince of Songkla U, Thailand)
2002-2008	Alexis Thompson	(PhD, 2008; Graduate College, UIUC)
2002-2007	Benjamin Levine	(PhD, 2007; Asst Prof, Michigan State)
2002-2008	Chaehyuk Ko	(PhD, 2008; Samsung, Korea)
2001-2004	Jane Owens	(PhD, 2004; Asst Prof, Central College, IA)
2001-2007	Joshua Coe	(PhD, 2007; Staff Scientist, Los Alamos National Lab)
2000-2007	James Hemp	(PhD, 2007; Postdoctoral, Cal Tech)
1997-2003	Seth Olsen	(PhD, 2004; ARC Fellow, Queensland U, Australia)
1997-2002	Jason Quenneville	(PhD, 2003; Senior Scientist, Spectral Sciences, MA)
1997-1999	Matthew Wander	(MS, 1999; Stony Brook, PhD 2007)
1997-1999	Dana Moore	(MS, 1999)

PUBLIC AND PROFESSIONAL SERVICE (SINCE 2012)

Co-Editor, Annual Reviews in Physical Chemistry (with Mark Johnson)	2011-present
Member, DOE Council on Chemical and Biochemical Sciences	2010-2015
Associate Editor, Journal of Chemical Physics	2007-present

UNIVERSITY, CAMPUS, AND DEPARTMENTAL SERVICE (Stanford and SLAC only)

Organizing committee, SLAC Faculty Retreat	2016
SLAC ALD Search Committee	2016
Chemistry Faculty Search Committee, Co-Chair	2016
Math-X Search Committee, Member	2016
Alliance for Graduate Education and the Professoriate (AGEP), Co-PI	2014-present
Enhancing Diversity in Graduate Education (EDGE), Faculty Mentor	2013-present
Raising Interest in Science and Engineering (RISE), Faculty Mentor	2012-present
Chair, LCLS SLAC/Stanford Search Committee	2012-present
Member, Academic Computing and Information Services (C-ACIS) Committee	2012-2015
Co-chair (w/ V. Pande), Stanford Research Computing Facility Committee	2010-present
Diversity Liaison, Chemistry	2009-present
Chair, SLAC Midrange Computing Committee	2009
Member, SLAC CIO Search Committee	2009

CONFERENCES CHAIRED AND ORGANIZED (SINCE 2012)

Chair, American Conference of Theoretical Chemistry	2020
Vice-Chair, American Conference of Theoretical Chemistry	2017

REVIEW PANELS

NIH Pioneer Award Reviewer, 2006, 2007, 2008
ACS Award Panel, 2004-2007
Department of Energy Panel Reviewer, 2002
National Science Foundation Panel Reviewer, 2000, 2004
Ad hoc reviewer for the following agencies, 1996-present:
Research Corporation; National Science Foundation; Petroleum Research Fund of the ACS; Department of Energy; Air Force Office of Scientific Research
Ad hoc reviewer for the following journals, 1996-present:
Journal of Chemical Physics; Journal of Physical Chemistry; Chemical Physics Letters; Chemical Physics; Journal of Molecular Structure; Langmuir; Steroids; Journal of the American Chemical Society; Physical Chemistry and Chemical Physics (PCCP); PhysChemComm; Inorganic Chemistry; Angewandte Chimie; Physical Review Letters; Proceedings of the National Academy of Sciences; Journal of Chemical Theory and Computation; Biophysica Biochimica Acta; Science; Nature; Nature Chemistry; Biophysical Journal

INVITED LECTURES SINCE 2012

DISTINGUISHED ADDRESSES

Keynote Lecturer, Computational Chemistry GRC, Girona, Spain	2016
Kroto Lecturer, Florida State University	2016
Keynote Lecturer, IUPAC-2015, Busan, South Korea	2015
Mulliken Lecturer, University of Georgia	2014
Inaugural Isaiah Shavitt Lecturer, Technion, Israel (Series of 4 lectures)	2014
MPS Distinguished Lecturer, National Science Foundation	2014
Xingda Lecturer, Peking University, China	2014
Plenary Lecturer, 22nd International Conference on Physical Organic Chemistry (ICPOC-22), Ottawa, Canada	2014
Gunning Lecturer, University of Alberta (Series of 3 Lectures)	2013
Albrecht Lecturer, Cornell University	2013
Distinguished Physical Chemistry Lecturer, University of Nevada, Reno (Series of 2 lectures)	2013

DEPARTMENTAL SEMINARS

California Institute of Technology	2016
University of Connecticut, Physics Colloquium	2016
Michigan State University	2016
Stockholm University, Stockholm, Sweden	2016
Uppsala University, Uppsala, Sweden	2015
Stockholm University, Stockholm, Sweden	2015
Linkoping University, Linkoping, Sweden	2015
Kyoto University	2015
University of Calgary	2015
Marmara University, Istanbul, Turkey	2015
Northwestern University	2014

Princeton University (Student-Selected Speaker)	2014
MIT/Harvard/Boston University Theoretical Chemistry Series	2014
University of Colorado, Boulder	2012
California Institute of Technology	2012

MEETINGS AND WORKSHOPS

10th MACCCR Fuel and Combustion Research Review, Chicago, IL	2016
Theory and Applications of Computational Chemistry (TACC), Seattle, WA	2016
Penn Conference on Theoretical Chemistry, Philadelphia, PA	2016
Workshop on Dynamical Quantum Effects in Molecular Processes, New York, NY	2016
9th International Meeting on Photodynamics, Mendoza, Argentina	2016
Shanghai International Symposium on Computational Chemistry, Shanghai, China	2015
1st Mueunjae Symposium on Chemistry and Light, POSTECH, Korea	2015
Workshop on "Excited States: Electronic Structure and Dynamics," Telluride, CO	2015
Workshop on "Quantum Effects in Condensed Phase Systems," Telluride, CO	2015
ACS Symposium on "Design Principles of Functional Macromolecular Materials", Denver, CO	2015
ACS Symposium on "Modeling Excited States of Complex Systems", Denver, CO	2015
ICQC Satellite Symposium on "Novel Computational Methods for Quantitative Electronic Structure Calculations," Kobe, Japan	2015
Dynamics of Molecular Collisions XXV, Asilomar, CA	2015
XL Congreso de Quimicos Teoricos de Expresion Latina, San Cristobal, Ecuador	2014
50th Symposium on Theoretical Chemistry, Vienna, Austria	2014
American Conference on Theoretical Chemistry (ACTC), Telluride, CO	2014
DAMOP Invited Session on "Non-Born-Oppenheimer Dynamics," Madison, WI	2014
LCLS/SSRL Workshop on "Characterizing and Controlling Chemical Dynamics," Menlo Park, CA	2014
LLNL Computational Chemistry and Materials Science Summer Institute	2014
Workshop on "Condensed Phase Dynamics," Telluride, CO	2014
ACS Symposium on "Quantum Mechanics in Many Dimensions," Indianapolis, IN	2013
ACS Symposium on "Frontiers in Reaction Dynamics," New Orleans, LA	2013
Third International Symposium on Computational Sciences, ISCS Shanghai, China	2013
SUNCAT Summer School, Menlo Park, CA	2013
Workshop on "Quantum Effects in Condensed Phase Systems," Telluride, CO	2013
CECAM Workshop on "Many-dimensional quantum dynamics with (non) classical trajectories," Lausanne, Switzerland	2013
Ultrafast X-Ray Summer School (UXSS), Hamburg, Germany	2013
Mathematical Methods in Quantum Molecular Dynamics, Banff, Canada	2013
CECAM Workshop on "High-Dimensional Quantum Dynamics," Birmingham, UK	2013
GRC on Atomic and Molecular Interactions, Easton, MA	2012
157th Faraday Discussion on Molecular Reaction Dynamics in Gases, Liquids and Interfaces, Assisi, Italy	2012
SimTech-CECAM Workshop on "Advanced Methods and Applications in Quantum Chemistry," Stuttgart, Germany	2012
Quantum Molecular Dynamics (Millefest), Berkeley, CA	2012
CUSO Summer School "From Electronic Structure to Quantum Dynamics," Villars, Switzerland (Series of 3 lectures)	2012

PROFESSIONAL SOCIETY MEMBERSHIPS

American Chemical Society
American Physical Society
American Association for the Advancement of Science
Biophysical Society

PEER-REVIEWED PUBLICATIONS

205. *Self-consistent Implementation of Ensemble Density Functional Theory Method for Multiple Strongly Correlated Electron Pairs*, M. Filatov, F. Liu, K. S. Kim, and T. J. Martínez, J. Chem. Phys., 145, 244104 (2016). DOI: 10.1063/1.4972174

204. *XFAIMS: eXternal Field Ab Initio Multiple Spawning for Electron-Nuclear Dynamics Triggered by Short Laser Pulses*, B. Mignolet, B. F. E. Curchod, and T. J. Martínez, J. Chem. Phys., 145, 191104 (2016). DOI: 10.1063/1.4967761

203. *Ab Initio Multiple Spawning Photochemical Dynamics of DMABN Using GPUs*, B. F. E. Curchod, A. Sisto, and T. J. Martínez, J. Phys. Chem. A, 121, 265-276 (2017). DOI: 10.1021/acs.jpca.6b09962

202. *How Large Should the QM Region be in QM/MM Calculations? The Case of Catechol O-Methyltransferase*, H. J. Kulik, J. Zhang, J. P. Klinman, and T. J. Martínez, J. Phys. Chem. B, 120, 11381-11394 (2016). Selected as ACS Editors' Choice. DOI: 10.1021/acs.jpcb.6b07814

201. *Pressure-Induced Neutral-to-Ionic Transition in an Amorphous Organic Material*, Y. Ren, S. Lee, J. M. Christensen, N. V. Plotnikov, M. Burgess, T. J. Martínez, D. D. Dlott, and J. S. Moore, Chem. Mat., 28, 6446-6449 (2016). DOI: 10.1021/acs.chemmater.6b02703

200. *Rich Athermal Ground-State Chemistry Triggered by Dynamics Through a Conical Intersection*, B. Mignolet, B. F. E. Curchod, and T. J. Martínez, Ang. Chem. Int. Ed., 55, 14993-14996 (2016). DOI: 10.1002/anie.201607633

199. *Molecular Origin of Mechanical Sensitivity of the Reaction Rate in Anthracene Cyclophane Isomerization Reveals Structural Motifs for Rational Design of Mechanophores*, N. Plotnikov and T. J. Martínez, J. Phys. Chem. C, 120, 17898-17908 (2016). DOI: 10.1021/acs.jpcc.6b04924

198. "*Balancing" the Block-Davidson-Liu Algorithm*, R. M. Parrish, E. G. Hohenstein, and T. J. Martínez, J. Chem. Theo. Comp., 12, 3003-3007 (2016). DOI: 10.1021/acs.jctc.6b00459

197. *Correction to "Toward Nonadiabatic Dynamics of Multichromophore Complexes: A Scalable GPU-Accelerated Exciton Framework"*, A. Sisto, D. R. Glowacki and T. J. Martínez, Acc. Chem. Res., 49, 1331 (2016).

196. *Comment on "Positive semidefinite tensor factorization of the two-electron integral matrix for low-scaling ab initio electronic structure" [J. Chem.Phys. 143 064103 (2015)]*, R. M. Parrish, E. G. Hohenstein, and T. J. Martínez, J. Chem. Phys., 145, 027101 (2016). DOI: 10.1063/1.4955316

195. *Adapting DFT+U for the Chemically-Motivated Correction of Minimal Basis Set Incompleteness*, H. J. Kulik, N. Seelam, B. D. Mar, and T. J. Martínez, J. Phys. Chem. A, 120, 5939-5949 (2016). DOI: 10.1021/acs.jpca.6b04527

194. *GPU-Accelerated State-Averaged Complete Active Space Self-Consistent Field Interfaced with Ab Initio Multiple Spawning Unravels the Photodynamics of Provitamin D_3*, J. W. Snyder Jr., B. F. E. Curchod, and T. J. Martínez, J. Phys. Chem. Lett., 7, 2444-2449 (2016). DOI: 10.1021/acs.jpclett.6b00970

193. *Toward Fully Quantum Modelling of Ultrafast Photodissociation Imaging Experiments. Treating Tunnelling in the Ab Initio Multiple Cloning Approach*, D. Makhov, T. J. Martínez, and D. Shalashilin, Faraday Disc., 194, 81-94 (2016). DOI: 10.1039/c6fd00073h

192. *Communication: A difference density picture for the self-consistent field ansatz*, R. M. Parrish, F. Liu, and T. J. Martínez, J. Chem. Phys., 144, 131101 (2016). DOI: 10.1063/1.4945277

191. *Atomic Orbital-Based SOS-MP2 with Tensor Hypercontraction: I. GPU-based Tensor Construction and Exploiting Sparsity*, C. Song and T. J. Martínez, J. Chem. Phys., 144, 174111 (2016). DOI: 10.1063/1.4948438

190. *Communication: GAIMS – Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes*, B. F. E. Curchod, C. Raue, P. Marquetand, L. Gonzalez, and T. J. Martínez, J. Chem. Phys., 144, 101102 (2016). DOI: 10.1063/1.4943571

189. *Using the GVB Ansatz to Develop Ensemble DFT Method for Describing Multiple Strongly Correlated Electron Pairs*, M. Filatov, T. J. Martínez and K. S. Kim, Phys. Chem. Chem. Phys., 18, 21040-21050 (2016). DOI: 10.1039/c6cp00236f

188. *Dynamical Correlation Effects on Photoisomerization: Ab Initio Multiple Spawning Dynamics with MS-CASPT2 for a Model trans-protonated Schiff Base*, L. Liu, J. Liu, and T. J. Martínez, J. Phys. Chem. B, 120, 1940-1949 (2016). DOI: 10.1021/acs.jpcb.5b09838

187. *Automated Code Engine for Graphical Processing Units: Application to Effective Core Potential Integrals and Gradients*, C. Song, L.-P. Wang, and T. J. Martínez, J. Chem. Theo. Comp., 12, 92-106 (2016). DOI: 10.1021/acs.jctc.5b00790

186. *Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways*, L.-P. Wang, R. T. McGibbon, V. S. Pande, and T. J. Martínez, J. Chem. Theo. Comp., 12, 638-649 (2016). DOI: 10.1021/acs.jctc.5b00830

185. *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*, J. W. Snyder, Jr., E. G. Hohenstein, N. Luehr, and T. J. Martínez, J. Chem. Phys., 143, 154107 (2015). DOI: 10.1063/1.4932613

184. *Ab Initio Interactive Molecular Dynamics on Graphical Processing Units (GPUs)*, N. Luehr, A. G. B. Jin, and T. J. Martínez, J. Chem. Theo. Comp., 11, 4536-4544 (2015). DOI: 10.1021/acs.jctc.5b00419

183. *Catch and Release: Orbital Symmetry Guided Reaction Dynamics from a Freed "Tension Trapped Transition State,"* Invited Article for Special Issue on "50 Years and Counting: The Woodward-Hoffmann Rules in the 21st Century," J. Wang, M. T. Ong, T. B. Kouznetsova, J. M. Lenhardt, T. J. Martínez, and S. L. Craig, J. Org. Chem., 80, 11773-11778 (2015). DOI: 10.1021/acs.joc.5b01493

182. *Ultrafast Isomerization Initiated by X-Ray Core Ionization*, C. Liekhus-Schmaltz, I. Tenney, T. Osipov, A. Sanchez-Gonzalez, N. Berrah, R. Boll, C. Bomme, C. Bostedt, J. Bozek, S. Carron, R. Coffee, J. Devin, B. Erk, K. Ferguson, R. Field, L. Foucar, L. Frasinski, J. Glownia, M. Guehr, A. Kamalov, J. Krzywinski, H. Li, J. Marangos, T. Martínez, B. McFarland, S. Miyabe, B. Murphy, A. Natan, D. Rolles, A. Rudenko, M. Siano, E. Simpson, L. Spector, M. Swiggers, D. Walke, S. Wang, T. Weber, P. Bucksbaum, and V. Petrovic, Nature Comm., 6, 8199 (2015). DOI: 10.1038/ncomms9199.

181. *Quantum chemical insights into the dependence of porphyrin basicity on the meso-aryl substituents: Thermodynamics, buckling, reaction sites and molecular flexibility*, M. Presselt, W. Dehaen, W. Maes, A. Klamt, T. Martínez, W. J. D. Beenken, and M. Kruk, Phys. Chem. Chem. Phys., 17, 14096-14106 (2015). DOI: 10.1039/C5CP01808K

180. *Origin of the Individual Basicity of Corrole NH-Tautomers: A Quantum Chemical Study on Molecular Structure and Dynamics, Kinetics, and Thermodynamics*, W. Beenken, W. Maes, M. Kruk, T. Martínez, and M. Presselt, J. Phys. Chem. A, 119, 6875-6883 (2015). DOI: 10.1021/acs.jpca.5b02869

179. *Determination of Hydrogen Bond Structure in Water versus Aprotic Environments to Test the Relationship Between Length and Stability*, P. A. Sigala, E. A. Ruben, C. W. Liu, P. M. B. Piccoli, E. G. Hohenstein, T. J. Martínez, A. J. Schulz, and D. Herschlag, J. Amer. Chem. Soc., 137, 5730-5740 (2015). DOI: 10.1021/ja512980h

178. *Efficient Implementation of Effective Core Potential Integrals and Gradients on Graphical Processing Units (GPUs)*, C. Song, L.-P. Wang, T. Sachse, J. Preiss, M. Presselt, and T. J. Martínez, J. Chem. Phys., 143, 014114 (2015). DOI: 10.1063/1.4922844

177. *Mediation of Donor-Acceptor Distance in an Enzymatic Methyl Transfer Reaction*, J. Zhang, H. J. Kulik, T. J. Martínez and J. P. Klinman, Proc. Natl. Acad. Sci., 112, 7954-7959 (2015). DOI: 10.1073/pnas.1506792112

176. *Ab Initio Multiple Spawning on Laser-Dressed States: A Study of 1,3-Cyclohexadiene Photoisomerization via Light-Induced Conical Intersections*, J. Kim, H. Tao, T. J. Martínez, and P. Bucksbaum, J. Phys. B, 48, 164003 (2015). DOI: 10.1088/0953-4075/48/16/164003

175. *Analytic First Derivatives of Floating Occupation Molecular Orbital-Complete Active Space Configuration Interaction on Graphical Processing Units*, E. G. Hohenstein, M. E. F. Bouduban, C. Song, N. Luehr, I. S. Ufimtsev and T. J. Martínez, J. Chem. Phys., 143, 014111 (2015). DOI: 10.1063/1.4923259

174. *Quantum Chemistry for Solvated Molecules on Graphical Processing Units (GPUs) using Polarizable Continuum Models*, F. Liu, N. Luehr, H. J. Kulik and T. J. Martínez, J. Chem. Theo. Comp., 11, 3131-3144 (2015). DOI: 10.1021/acs.jctc.5b00370

173. *Tensor hypercontraction second-order Moller-Plesset Perturbation Theory: Grid Optimization and Reaction Energies*, S. I. L. Kokkila Schumacher, E. G. Hohenstein, R. M. Parrish, L.-P. Wang, and T. J. Martínez, J. Chem. Theo. Comp., 11, 3042-3052 (2015). DOI: 10.1021/acs.jctc.5b00272

172. *An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units*, E. G. Hohenstein, N. Luehr, I. S. Ufimtsev, and T. J. Martínez, J. Chem. Phys., 142, 224103 (2015). DOI: 10.1063/1.4921956

171. *How does peripheral functionalization of Ruthenium(II)-Terpyridine Complexes affect spatial charge redistribution after photoexcitation at the Franck-Condon point?*, J. Preiss, M. Jager, S. Rau, B. Dietzek, J. Popp. T. Martínez, and M. Presselt, ChemPhysChem, 16, 1395-1404 (2015). DOI: 10.1002/cphc.201500223

170. *Inducing and quantifying forbidden reactivity with single-molecule polymer mechanochemistry*, J. Wang, T. B. Kouznetsova, Z. Niu, M. T. Ong, H. M. Klukovich, A. L. Rheingold, T. J. Martínez, and S. L. Craig, Nature Chem. 7, 323-327 (2015). DOI: 10.1038/nchem.2185

169. *Ab Initio Multiple Cloning Simulations of Pyrrole Photodissociation: TKER Spectra and Velocity Map Imaging*, D. Makhov, K. Saita, T. J. Martínez, and D. V. Shalashilin, Phys. Chem. Chem. Phys., 17 3316-3325 (2015). DOI: 10.1039/c4cp04571h

168. *Direct QM/MM Excited State Dynamics of Retinal Protonated Schiff Base in Isolation and Methanol Solution*, C. Punwong, J. Owens, and T. J. Martínez, J. Phys. Chem. B, 119, 704-714 (2015). DOI: 10.1021/jp5038798

167. *A Remote Stereochemical Lever Arm Effect in Polymer Mechanochemistry*, J. Wang, T. B. Kouznetsova, Z. S. Kean, L. Fan, B. D. Mar, T. J. Martínez, and S. L. Craig, J. Amer. Chem. Soc. **136**, 15162-15165 (2014).

166. *Interfacing the Ab Initio Multiple Spawning Method with Electronic Structure Methods in GAMESS: Photo-decay of trans-azomethane*, A. Gaenko, A. DeFusco, S. A. Varganov, T. J. Martínez, and M. S. Gordon, J. Phys. Chem. A, 118 (46), 10902–10908 (2014). DOI: 10.1021/jp508242j

165. *Ab Initio Nonadiabatic Dynamics of Multichromophore Complexes: A Scalable GPU-Accelerated Exciton Framework,* A. Sisto, D. R. Glowacki, and T. J. Martínez, *Acc. Chem. Res.*, **47**, 2857-2866 (2014). DOI: 10.1021/ar500229p

164. *Direct QM/MM Simulation of Photoexcitation Dynamics in Bacteriorhodopsin and Halorhodopsin*, C. Punwong, T. J. Martínez, and S. Hannongbua, Chem. Phys. Lett., **610**, 213-218 (2014). DOI: 10.1016/j.cplett.2014.07.037

163. *Steric and Electronic Contributions to the Core Reactivity of Monoprotonated 5-phenylporphyrin: A DFT Study*, M. Presselt, M. Wojdyr, W. J. D. Beenken, M. Kruk, and T. J. Martínez, Chem. Phys. Lett., **603**, 21-27 (2014). DOI: 10.1016/j.cplett.2014.04.011

162. *Ultrafast X-Ray Auger Probing of Photoexcited Molecular Dynamics*, B. K. McFarland, J. P. Farrell, S. Miyabe, F. Tarantelli, A. Aguilar, N. Berrah, C. Bostedt, J. D. Bozek, P. H. Bucksbaum, J. C. Castagna, R. N. Coffee, J. P. Cryan, L. Fang, R. Feifel, K. J. Gaffney, J. M. Glownia, T. J. Martínez, M. Mucke, B. Murphy, A. Natan, T. Osipov, V. S. Petrovic, S. Schorb, Th. Schultz, L. S. Spector, M. Swiggers, I. Tenney, S. Wang, J. L. White, W. White, and M. Guehr, Nature Comm., **5**, 4235 (2014). DOI: 10.1038/ncomms5235

161. *Gaussian Basis Set Hartree-Fock, Density Functional Theory and Beyond on GPUs*, N. Luehr, A. Sisto, and T. J. Martínez in Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics, Ed. R. C. Walker and A. W. Goetz (Chichester, Wiley, 2016) p. 67-100.

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