Todd J Martinez

List of Publications by Year in Descending Order

304 papers	19,947 citations	76 h-index	131 g-index
353 ext. papers	22,290 ext. citations	7.2 avg, IF	7.31 L-index

#	Paper	IF	Citations
304	Internal conversion of the anionic GFP chromophore: in and out of the I-twisted S/S conical intersection seam.. *Chemical Science*, **2022**, 13, 373-385	9.4	3
303	Rank-reduced coupled-cluster. III. Tensor hypercontraction of the doubles amplitudes.. *Journal of Chemical Physics*, **2022**, 156, 054102	3.9	4
302	Chiral photochemistry of achiral molecules.. *Nature Communications*, **2022**, 13, 2091	17.4	1
301	Proton Transfer from a Photoacid to a Water Wire: First Principles Simulations and Fast Fluorescence Spectroscopy. *Journal of Physical Chemistry B*, **2021**, 125, 12539-12551	3.4	3
300	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*, **2021**, 143, 20015-20021	16.4	5
299	GPU acceleration of rank-reduced coupled-cluster singles and doubles. *Journal of Chemical Physics*, **2021**, 155, 184110	3.9	2
298	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *Journal of Chemical Physics*, **2021**, 155, 204801	3.9	3
297	Conformer-specific photochemistry imaged in real space and time. *Science*, **2021**, 374, 178-182	33.3	2
296	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*, **2021**, 17, 7120-7133	6.4	0
295	A Tribute to Emily A. Carter. *Journal of Physical Chemistry A*, **2021**, 125, 1669-1670	2.8	
294	Substituent Effects in Mechanochemical Allowed and Forbidden Cyclobutene Ring-Opening Reactions. *Journal of the American Chemical Society*, **2021**, 143, 3846-3855	16.4	4
293	Comparing (stochastic-selection) ab initio multiple spawning with trajectory surface hopping for the photodynamics of cyclopropanone, fulvene, and dithiane. *Journal of Chemical Physics*, **2021**, 154, 104110	3.9	10
292	Parallel molecular mechanisms for enzyme temperature adaptation. *Science*, **2021**, 371,	33.3	11
291	Analytical derivatives of the individual state energies in ensemble density functional theory. II. Implementation on graphical processing units (GPUs). *Journal of Chemical Physics*, **2021**, 154, 104108	3.9	4
290	A Tribute to Emily A. Carter. *Journal of Physical Chemistry C*, **2021**, 125, 4331-4332	3.8	
289	Electrostatic Control of Photoisomerization in Channelrhodopsin 2. *Journal of the American Chemical Society*, **2021**, 143, 5425-5437	16.4	2
288	Unmasking the -Stilbene Phantom State via Vacuum Ultraviolet Time-Resolved Photoelectron Spectroscopy and Multiple Spawning. *Journal of Physical Chemistry Letters*, **2021**, 12, 6363-6369	6.4	2

287	Understanding the Mechanochemistry of Ladder-Type Cyclobutane Mechanophores by Single Molecule Force Spectroscopy. *Journal of the American Chemical Society*, **2021**, 143, 12328-12334	16.4	11
286	Flyby reaction trajectories: Chemical dynamics under extrinsic force. *Science*, **2021**, 373, 208-212	33.3	8
285	A diagrammatic approach for automatically deriving analytical gradients of tensor hyper-contracted electronic structure methods. *Journal of Chemical Physics*, **2021**, 155, 024108	3.9	0
284	TeraChem: A graphical processing unit-accelerated electronic structure package for large-scale ab initio molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1494	7.9	49
283	Reduced scaling formulation of CASPT2 analytical gradients using the supporting subspace method. *Journal of Chemical Physics*, **2021**, 154, 014103	3.9	7
282	The non-adiabatic nanoreactor: towards the automated discovery of photochemistry. *Chemical Science*, **2021**, 12, 7294-7307	9.4	6
281	Voice-controlled quantum chemistry. *Nature Computational Science*, **2021**, 1, 42-45		3
280	Nitromethane Decomposition via Automated Reaction Discovery and an Corrected Kinetic Model. *Journal of Physical Chemistry A*, **2021**, 125, 1447-1460	2.8	1
279	Cover Image, Volume 11, Issue 2. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1523	7.9	3
278	Direct observation of ultrafast hydrogen bond strengthening in liquid water. *Nature*, **2021**, 596, 531-535	50.4	13
277	Resolving the ultrafast dynamics of the anionic green fluorescent protein chromophore in water. *Chemical Science*, **2021**, 12, 11347-11363	9.4	3
276	Transient resonant Auger-Meitner spectra of photoexcited thymine. *Faraday Discussions*, **2021**, 228, 555-570	3.7	2
275	ChemPix: automated recognition of hand-drawn hydrocarbon structures using deep learning. *Chemical Science*, **2021**, 12, 10622-10633	9.4	3
274	Fast transformations between configuration state function and Slater determinant bases for direct configuration interaction. *Journal of Chemical Physics*, **2020**, 152, 164111	3.9	5
273	Strictly non-adiabatic quantum control of the acetylene dication using an infrared field. *Journal of Chemical Physics*, **2020**, 152, 184302	3.9	1
272	Nonadiabatic Dynamics of Photoexcited -Stilbene Using Ab Initio Multiple Spawning. *Journal of Physical Chemistry B*, **2020**, 124, 5476-5487	3.4	8
271	Simultaneous observation of nuclear and electronic dynamics by ultrafast electron diffraction. *Science*, **2020**, 368, 885-889	33.3	43
270	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. *Journal of Chemical Physics*, **2020**, 152, 224110	3.9	40

269	Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures. *Journal of Chemical Theory and Computation*, **2020**, 16, 4021-4028	6.4	11
268	Reduced scaling extended multi-state CASPT2 (XMS-CASPT2) using supporting subspaces and tensor hyper-contraction. *Journal of Chemical Physics*, **2020**, 152, 234113	3.9	9
267	Matter-wave interference of a native polypeptide. *Nature Communications*, **2020**, 11, 1447	17.4	14
266	Strong, Nonresonant Radiation Enhances - Photoisomerization of Stilbene in Solution. *Journal of Physical Chemistry A*, **2020**, 124, 5999-6008	2.8	3
265	SSAIMS-Stochastic-Selection Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. *Journal of Physical Chemistry A*, **2020**, 124, 6133-6143	2.8	10
264	The cascade unzipping of ladderane reveals dynamic effects in mechanochemistry. *Nature Chemistry*, **2020**, 12, 302-309	17.6	48
263	The Mechanics of the Bicycle Pedal Photoisomerization in Crystalline -1,4-Diphenyl-1,3-butadiene. *Journal of Physical Chemistry A*, **2020**, 124, 8897-8906	2.8	2
262	Intermolecular vibrations mediate ultrafast singlet fission. *Science Advances*, **2020**, 6,	14.3	19
261	Hole-hole Tamm-Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. *Journal of Chemical Physics*, **2020**, 153, 024110	3.9	15
260	Efficient Treatment of Large Active Spaces through Multi-GPU Parallel Implementation of Direct Configuration Interaction. *Journal of Chemical Theory and Computation*, **2020**, 16, 1586-1596	6.4	13
259	Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the n□ and □ Excited States. *Journal of the American Chemical Society*, **2020**, 142, 20680-20690	16.4	20
258	An ab initio exciton model for singlet fission. *Journal of Chemical Physics*, **2020**, 153, 184116	3.9	5
257	A multilayer multi-configurational approach to efficiently simulate large-scale circuit-based quantum computers on classical machines. *Journal of Chemical Physics*, **2020**, 153, 051101	3.9	2
256	Nonadiabatic Molecular Dynamics with Hole-Hole Tamm-Dancoff Approximated Density Functional Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 5499-5511	6.4	12
255	PySpawn: Software for Nonadiabatic Quantum Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2020**, 16, 5485-5498	6.4	5
254	Proton Transfer Dynamics in the Aprotic Proton Accepting Solvent 1-Methylimidazole. *Journal of Physical Chemistry B*, **2020**, 124, 7897-7908	3.4	4
253	Putting Photomechanical Switches to Work: An Multiple Spawning Study of Donor-Acceptor Stenhouse Adducts. *Journal of Physical Chemistry Letters*, **2020**, 11, 7901-7907	6.4	11
252	TeraChem Cloud: A High-Performance Computing Service for Scalable Distributed GPU-Accelerated Electronic Structure Calculations. *Journal of Chemical Information and Modeling*, **2020**, 60, 2126-2137	6.1	11

251	Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy. *Chemical Science*, **2020**, 11, 4180-4193	9.4	11
250	Diffractive imaging of dissociation and ground-state dynamics in a complex molecule. *Physical Review A*, **2019**, 100,	2.6	15
249	Imaging the ring opening reaction of 1,3-cyclohexadiene with MeV ultrafast electron diffraction. *EPJ Web of Conferences*, **2019**, 205, 07006	0.3	
248	Sub-Femtosecond Stark Control of Molecular Photoexcitation with Near Single-Cycle Pulses. *Journal of Physical Chemistry Letters*, **2019**, 10, 742-747	6.4	7
247	Ab Initio Computation of Rotationally-Averaged Pump-Probe X-ray and Electron Diffraction Signals. *Journal of Chemical Theory and Computation*, **2019**, 15, 1523-1537	6.4	13
246	Multicolor Mechanochromism of a Polymer/Silica Composite with Dual Distinct Mechanophores. *Journal of the American Chemical Society*, **2019**, 141, 1898-1902	16.4	74
245	Perturbation of Short Hydrogen Bonds in Photoactive Yellow Protein via Noncanonical Amino Acid Incorporation. *Journal of Physical Chemistry B*, **2019**, 123, 4844-4849	3.4	7
244	Electrostatic Influence on Photoisomerization in Bacteriorhodopsin and Halorhodopsin. *Journal of Physical Chemistry B*, **2019**, 123, 4850-4857	3.4	3
243	Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver. *Physical Review Letters*, **2019**, 122, 230401	7.4	78
242	Nonadiabatic Photodynamics of Retinal Protonated Schiff Base in Channelrhodopsin 2. *Journal of Physical Chemistry Letters*, **2019**, 10, 2862-2868	6.4	16
241	Rank reduced coupled cluster theory. I. Ground state energies and wavefunctions. *Journal of Chemical Physics*, **2019**, 150, 164118	3.9	20
240	The photochemical ring-opening of 1,3-cyclohexadiene imaged by ultrafast electron diffraction. *Nature Chemistry*, **2019**, 11, 504-509	17.6	100
239	Geodesic interpolation for reaction pathways. *Journal of Chemical Physics*, **2019**, 150, 164103	3.9	20
238	Reaction Dynamics of Cyanohydrins with Hydrosulfide in Water. *Journal of Physical Chemistry A*, **2019**, 123, 7210-7217	2.8	4
237	On combining the conductor-like screening model and optimally tuned range-separated hybrid density functionals. *Journal of Chemical Physics*, **2019**, 150, 174117	3.9	6
236	Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy. *Journal of Physical Chemistry A*, **2019**, 123, 6897-6903	2.8	19
235	Disentangling conical intersection and coherent molecular dynamics in methyl bromide with attosecond transient absorption spectroscopy. *Nature Communications*, **2019**, 10, 3133	17.4	40
234	Photo-protection/photo-damage in natural systems: general discussion. *Faraday Discussions*, **2019**, 216, 538-563	3.6	4

233	Photovoltaics and bio-inspired light harvesting: general discussion. *Faraday Discussions*, **2019**, 216, 269-306	3.6	
232	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*, **2019**, 141, 18193-18203	16.4	28
231	Relaxation Dynamics of Hydrated Thymine, Thymidine, and Thymidine Monophosphate Probed by Liquid Jet Time-Resolved Photoelectron Spectroscopy. *Journal of Physical Chemistry A*, **2019**, 123, 10676-10684	2.8	11
230	Rank reduced coupled cluster theory. II. Equation-of-motion coupled-cluster singles and doubles. *Journal of Chemical Physics*, **2019**, 151, 164121	3.9	6
229	Exploiting graphical processing units to enable quantum chemistry calculation of large solvated molecules with conductor-like polarizable continuum models. *International Journal of Quantum Chemistry*, **2019**, 119, e25760	2.1	23
228	Ab Initio Nonadiabatic Quantum Molecular Dynamics. *Chemical Reviews*, **2018**, 118, 3305-3336	68.1	321
227	Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. I. Time-resolved photoelectron-photoion coincidence spectroscopy. *Journal of Chemical Physics*, **2018**, 148, 164302	3.9	28
226	Large-Scale Functional Group Symmetry-Adapted Perturbation Theory on Graphical Processing Units. *Journal of Chemical Theory and Computation*, **2018**, 14, 1737-1753	6.4	13
225	Nonadiabatic Ab Initio Molecular Dynamics with the Floating Occupation Molecular Orbital-Complete Active Space Configuration Interaction Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 339-350	6.4	41
224	A program for automatically predicting supramolecular aggregates and its application to urea and porphin. *Journal of Computational Chemistry*, **2018**, 39, 763-772	3.5	8
223	Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. II. Ab initio multiple spawning simulations. *Journal of Chemical Physics*, **2018**, 148, 164303	3.9	37
222	Mixed quantum-classical electrodynamics: Understanding spontaneous decay and zero-point energy. *Physical Review A*, **2018**, 97,	2.6	23
221	Reduced scaling CASPT2 using supporting subspaces and tensor hyper-contraction. *Journal of Chemical Physics*, **2018**, 149, 044108	3.9	23
220	Structural Coupling Throughout the Active Site Hydrogen Bond Networks of Ketosteroid Isomerase and Photoactive Yellow Protein. *Journal of the American Chemical Society*, **2018**, 140, 9827-9843	16.4	23
219	Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. *Journal of Chemical Theory and Computation*, **2018**, 14, 4139-4150	6.4	21
218	Ab Initio Prediction of Fluorescence Lifetimes Involving Solvent Environments by Means of COSMO and Vibrational Broadening. *Journal of Physical Chemistry A*, **2018**, 122, 9813-9820	2.8	4
217	Photoannealing of Merocyanine Aggregates. *Journal of Physical Chemistry A*, **2018**, 122, 9821-9832	2.8	5
216	Imaging CFI conical intersection and photodissociation dynamics with ultrafast electron diffraction. *Science*, **2018**, 361, 64-67	33.3	117

215	Atomistic non-adiabatic dynamics of the LH2 complex with a GPU-accelerated ab initio exciton model. *Physical Chemistry Chemical Physics*, **2017**, 19, 14924-14936	3.6	48
214	A direct-compatible formulation of the coupled perturbed complete active space self-consistent field equations on graphical processing units. *Journal of Chemical Physics*, **2017**, 146, 174113	3.9	37
213	An Ab Initio Exciton Model Including Charge-Transfer Excited States. *Journal of Chemical Theory and Computation*, **2017**, 13, 3493-3504	6.4	66
212	Atomic orbital-based SOS-MP2 with tensor hypercontraction. II. Local tensor hypercontraction. *Journal of Chemical Physics*, **2017**, 146, 034104	3.9	22
211	CASSCF: An Efficient, Empirical Correction for SA-CASSCF To Closely Approximate MS-CASPT2 Potential Energy Surfaces. *Journal of Physical Chemistry Letters*, **2017**, 8, 2432-2437	6.4	23
210	Probing ultrafast /n internal conversion in organic chromophores via K-edge resonant absorption. *Nature Communications*, **2017**, 8, 29	17.4	101
209	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. *Journal of Physical Chemistry B*, **2017**, 121, 4023-4039	3.4	147
208	Ab Initio Reactive Computer Aided Molecular Design. *Accounts of Chemical Research*, **2017**, 50, 652-656	24.3	31
207	Ab Initio Multiple Spawning Photochemical Dynamics of DMABN Using GPUs. *Journal of Physical Chemistry A*, **2017**, 121, 265-276	2.8	43
206	Absorption and Fluorescence Features of an Amphiphilic meso-Pyrimidinylcorrole: Experimental Study and Quantum Chemical Calculations. *Journal of Physical Chemistry A*, **2017**, 121, 8614-8624	2.8	11
205	Pomeranz-Fritsch Synthesis of Isoquinoline: Gas-Phase Collisional Activation Opens Additional Reaction Pathways. *Journal of the American Chemical Society*, **2017**, 139, 14352-14355	16.4	12
204	Ultrafast isomerization in acetylene dication after carbon K-shell ionization. *Nature Communications* , **2017**, 8, 453	17.4	20
203	Analytical gradients for tensor hyper-contracted MP2 and SOS-MP2 on graphical processing units. *Journal of Chemical Physics*, **2017**, 147, 161723	3.9	14
202	Analytical derivatives of the individual state energies in ensemble density functional theory method. I. General formalism. *Journal of Chemical Physics*, **2017**, 147, 034113	3.9	42
201	The Spin-Flip Variant of the Algebraic-Diagrammatic Construction Yields the Correct Topology of S/S Conical Intersections. *Journal of Chemical Theory and Computation*, **2017**, 13, 4436-4441	6.4	22
200	Mechanochemical unzipping of insulating polyladderene to semiconducting polyacetylene. *Science*, **2017**, 357, 475-479	33.3	175
199	Description of ground and excited electronic states by ensemble density functional method with extended active space. *Journal of Chemical Physics*, **2017**, 147, 064104	3.9	23
198	Crossing conditions in coupled cluster theory. *Journal of Chemical Physics*, **2017**, 147, 164105	3.9	31

197	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*, **2017**, 13, 6230-6236	6.4	22
196	Probing molecular photoinduced dynamics by ultrafast soft x-rays **2017**,		1
195	Observing Femtosecond Fragmentation Using Ultrafast X-ray-Induced Auger Spectra. *Applied Sciences (Switzerland)*, **2017**, 7, 681	2.6	15
194	Toward fully quantum modelling of ultrafast photodissociation imaging experiments. Treating tunnelling in the ab initio multiple cloning approach. *Faraday Discussions*, **2016**, 194, 81-94	3.6	23
193	Pressure-Induced Neutral-to-Ionic Transition in an Amorphous Organic Material. *Chemistry of Materials*, **2016**, 28, 6446-6449	9.6	2
192	Gaussian Basis Set HartreeFock, Density Functional Theory, and Beyond on GPUs **2016**, 67-100		3
191	Rich Athermal Ground-State Chemistry Triggered by Dynamics through a Conical Intersection. *Angewandte Chemie - International Edition*, **2016**, 55, 14993-14996	16.4	19
190	"Balancing" the Block Davidson-Liu Algorithm. *Journal of Chemical Theory and Computation*, **2016**, 12, 3003-7	6.4	18
189	GPU-Accelerated State-Averaged Complete Active Space Self-Consistent Field Interfaced with Ab Initio Multiple Spawning Unravels the Photodynamics of Provitamin D3. *Journal of Physical Chemistry Letters*, **2016**, 7, 2444-9	6.4	47
188	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*, **2016**, 120, 1940-9	3.4	53
187	Automated Code Engine for Graphical Processing Units: Application to the Effective Core Potential Integrals and Gradients. *Journal of Chemical Theory and Computation*, **2016**, 12, 92-106	6.4	46
186	Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. *Physical Chemistry Chemical Physics*, **2016**, 18, 21040-50	3.6	18
185	Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways. *Journal of Chemical Theory and Computation*, **2016**, 12, 638-49	6.4	73
184	Transient NEXAFS Spectroscopy at the Oxygen Edge: Pinning Down π/nπ Internal Conversion **2016**,		1
183	Adapting DFT+U for the Chemically Motivated Correction of Minimal Basis Set Incompleteness. *Journal of Physical Chemistry A*, **2016**, 120, 5939-49	2.8	16
182	Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. *Journal of Chemical Physics*, **2016**, 145, 244104	3.9	21
181	Communication: A difference density picture for the self-consistent field ansatz. *Journal of Chemical Physics*, **2016**, 144, 131101	3.9	4
180	Communication: GAIMS--Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. *Journal of Chemical Physics*, **2016**, 144, 101102	3.9	74

179	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*, **2016**, 145, 027101	3.9	1
178	Atomic orbital-based SOS-MP2 with tensor hypercontraction. I. GPU-based tensor construction and exploiting sparsity. *Journal of Chemical Physics*, **2016**, 144, 174111	3.9	38
177	Communication: XFAIMS-eXternal Field Ab Initio Multiple Spawning for electron-nuclear dynamics triggered by short laser pulses. *Journal of Chemical Physics*, **2016**, 145, 191104	3.9	28
176	Rich Athermal Ground-State Chemistry Triggered by Dynamics through a Conical Intersection. *Angewandte Chemie*, **2016**, 128, 15217-15220	3.6	8
175	How Large Should the QM Region Be in QM/MM Calculations? The Case of Catechol O-Methyltransferase. *Journal of Physical Chemistry B*, **2016**, 120, 11381-11394	3.4	110
174	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*, **2016**, 120, 17898-17908	3.8	11
173	Inducing and quantifying forbidden reactivity with single-molecule polymer mechanochemistry. *Nature Chemistry*, **2015**, 7, 323-7	17.6	141
172	Quantum Chemistry for Solvated Molecules on Graphical Processing Units Using Polarizable Continuum Models. *Journal of Chemical Theory and Computation*, **2015**, 11, 3131-44	6.4	69
171	Mediation of donor-acceptor distance in an enzymatic methyl transfer reaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 7954-9	11.5	55
170	Determination of Hydrogen Bond Structure in Water versus Aprotic Environments To Test the Relationship Between Length and Stability. *Journal of the American Chemical Society*, **2015**, 137, 5730-40	16.4	43
169	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*, **2015**, 17, 14096-106	3.6	27
168	An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units. *Journal of Chemical Physics*, **2015**, 142, 224103	3.9	83
167	Ab initiomultiple 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*, **2015**, 48, 164003	1.3	38
166	Ab initio interactive molecular dynamics on graphical processing units (GPUs). *Journal of Chemical Theory and Computation*, **2015**, 11, 4536-44	6.4	37
165	Catch and Release: Orbital Symmetry Guided Reaction Dynamics from a Freed "Tension Trapped Transition State". *Journal of Organic Chemistry*, **2015**, 80, 11773-8	4.2	13
164	Ultrafast isomerization initiated by X-ray core ionization. *Nature Communications*, **2015**, 6, 8199	17.4	74
163	Ab initio multiple cloning simulations of pyrrole photodissociation: TKER spectra and velocity map imaging. *Physical Chemistry Chemical Physics*, **2015**, 17, 3316-25	3.6	60
162	Efficient implementation of effective core potential integrals and gradients on graphical processing units. *Journal of Chemical Physics*, **2015**, 143, 014114	3.9	13

161	Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units. *Journal of Chemical Physics*, **2015**, 143, 014111	3.9	35
160	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*, **2015**, 143, 154107	3.9	52
159	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. *Journal of Chemical Physics*, **2015**, 143, 102601	3.9	10
158	How Does Peripheral Functionalization of Ruthenium(II)-Terpyridine Complexes Affect Spatial Charge Redistribution after Photoexcitation at the Franck-Condon Point?. *ChemPhysChem*, **2015**, 16, 1395-404	3.2	31
157	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*, **2015**, 119, 6875-83	2.8	18
156	Tensor Hypercontraction Second-Order Møller-Plesset Perturbation Theory: Grid Optimization and Reaction Energies. *Journal of Chemical Theory and Computation*, **2015**, 11, 3042-52	6.4	38
155	Direct QM/MM excited-state dynamics of retinal protonated Schiff base in isolation and methanol solution. *Journal of Physical Chemistry B*, **2015**, 119, 704-14	3.4	28
154	Time-Resolved Photoelectron Spectroscopy and Ab Initio Multiple Spawning Studies of Hexamethylcyclopentadiene. *Springer Proceedings in Physics*, **2015**, 184-187	0.2	
153	Axis-dependence of molecular high harmonic emission in three dimensions. *Nature Communications* , **2014**, 5, 3190	17.4	16
152	Modeling mechanophore activation within a viscous rubbery network. *Journal of the Mechanics and Physics of Solids*, **2014**, 63, 141-153	5	42
151	Multiple time step integrators in ab initio molecular dynamics. *Journal of Chemical Physics*, **2014**, 140, 084116	3.9	32
150	Discovering chemistry with an ab initio nanoreactor. *Nature Chemistry*, **2014**, 6, 1044-8	17.6	209
149	A remote stereochemical lever arm effect in polymer mechanochemistry. *Journal of the American Chemical Society*, **2014**, 136, 15162-5	16.4	72
148	Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations. *Physical Chemistry Chemical Physics*, **2014**, 16, 11770-9	3.6	33
147	Direct QM/MM simulation of photoexcitation dynamics in bacteriorhodopsin and halorhodopsin. *Chemical Physics Letters*, **2014**, 610-611, 213-218	2.5	15
146	Photochemical Dynamics of Ethylene Cation C2H4(.). *Journal of Physical Chemistry Letters*, **2014**, 5, 1467-71	6.1	27
145	Steric and electrostatic effects on photoisomerization dynamics using QM/MM ab initio multiple spawning. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	19
144	Ab initio nonadiabatic dynamics of multichromophore complexes: a scalable graphical-processing-unit-accelerated exciton framework. *Accounts of Chemical Research*, **2014**, 47, 2857-66	24.3	73

143	Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer. *Nature Chemistry*, **2014**, 6, 623-8	17.6	157
142	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 1885-91	6.4	294
141	Steric and electronic contributions to the core reactivity of monoprotonated 5-phenylporphyrin: A DFT study. *Chemical Physics Letters*, **2014**, 603, 21-27	2.5	12
140	Ultrafast X-ray Auger probing of photoexcited molecular dynamics. *Nature Communications*, **2014**, 5, 4235	17.4	117
139	Experimental strategies for optical pump soft x-ray probe experiments at the LCLS. *Journal of Physics: Conference Series*, **2014**, 488, 012015	0.3	15
138	Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics. *Journal of Chemical Physics*, **2014**, 141, 054110	3.9	135
137	Communication: Acceleration of coupled cluster singles and doubles via orbital-weighted least-squares tensor hypercontraction. *Journal of Chemical Physics*, **2014**, 140, 181102	3.9	48
136	Interfacing the Ab initio multiple spawning method with electronic structure methods in GAMESS: Photodecay of trans-azomethane. *Journal of Physical Chemistry A*, **2014**, 118, 10902-8	2.8	25
135	Systematic improvement of a classical molecular model of water. *Journal of Physical Chemistry B*, **2013**, 117, 9956-72	3.4	235
134	Generating Efficient Quantum Chemistry Codes for Novel Architectures. *Journal of Chemical Theory and Computation*, **2013**, 9, 213-21	6.4	226
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