Todd J Martinez

List of Publications by Citations

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	Force-induced activation of covalent bonds in mechanoresponsive polymeric materials. *Nature*, **2009**, 459, 68-72	50.4	1211
303	Isomerization through conical intersections. *Annual Review of Physical Chemistry*, **2007**, 58, 613-34	15.7	659
302	Ab Initio Multiple Spawning: Photochemistry from First Principles Quantum Molecular Dynamics. *Journal of Physical Chemistry A*, **2000**, 104, 5161-5175	2.8	627
301	Quantum Chemistry on Graphical Processing Units. 3. Analytical Energy Gradients, Geometry Optimization, and First Principles Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2009**, 5, 2619-28	6.4	585
300	Conical intersections and double excitations in time-dependent density functional theory. *Molecular Physics*, **2006**, 104, 1039-1051	1.7	479
299	Quantum Chemistry on Graphical Processing Units. 1. Strategies for Two-Electron Integral Evaluation. *Journal of Chemical Theory and Computation*, **2008**, 4, 222-31	6.4	373
298	Multi-Electronic-State Molecular Dynamics: A Wave Function Approach with Applications. *The Journal of Physical Chemistry*, **1996**, 100, 7884-7895		335
297	Ab Initio Nonadiabatic Quantum Molecular Dynamics. *Chemical Reviews*, **2018**, 118, 3305-3336	68.1	321
296	Ab initio molecular dynamics and time-resolved photoelectron spectroscopy of electronically excited uracil and thymine. *Journal of Physical Chemistry A*, **2007**, 111, 8500-8	2.8	316
295	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 1885-91	6.4	294
294	Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field Implementation. *Journal of Chemical Theory and Computation*, **2009**, 5, 1004-15	6.4	291
293	Optimizing conical intersections without derivative coupling vectors: application to multistate multireference second-order perturbation theory (MS-CASPT2). *Journal of Physical Chemistry B*, **2008**, 112, 405-13	3.4	288
292	Mechanism and dynamics of azobenzene photoisomerization. *Journal of the American Chemical Society*, **2003**, 125, 8098-9	16.4	261
291	Ab Initio Quantum Molecular Dynamics. *Advances in Chemical Physics*, **2002**, 439-512		260
290	Photodynamics in complex environments: ab initio multiple spawning quantum mechanical/molecular mechanical dynamics. *Journal of Physical Chemistry B*, **2009**, 113, 3280-91	3.4	246
289	Trapping a diradical transition state by mechanochemical polymer extension. *Science*, **2010**, 329, 1057-60	33.3	241
288	Systematic improvement of a classical molecular model of water. *Journal of Physical Chemistry B*, **2013**, 117, 9956-72	3.4	235

287	Generating Efficient Quantum Chemistry Codes for Novel Architectures. *Journal of Chemical Theory and Computation*, **2013**, 9, 213-21	6.4	226
286	Ab Initio Study of Cis□trans Photoisomerization in Stilbene and Ethylene. *Journal of Physical Chemistry A*, **2003**, 107, 829-837	2.8	225
285	Conical intersection dynamics in solution: the chromophore of Green Fluorescent Protein. *Faraday Discussions*, **2004**, 127, 149-63	3.6	213
284	Discovering chemistry with an ab initio nanoreactor. *Nature Chemistry*, **2014**, 6, 1044-8	17.6	209
283	Insights for light-driven molecular devices from ab initio multiple spawning excited-state dynamics of organic and biological chromophores. *Accounts of Chemical Research*, **2006**, 39, 119-26	24.3	196
282	First principles dynamics and minimum energy pathways for mechanochemical ring opening of cyclobutene. *Journal of the American Chemical Society*, **2009**, 131, 6377-9	16.4	178
281	Tensor hypercontraction density fitting. I. Quartic scaling second- and third-order M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2012**, 137, 044103	3.9	176
280	Mechanochemical unzipping of insulating polyladderene to semiconducting polyacetylene. *Science*, **2017**, 357, 475-479	33.3	175
279	Implementation of ab initio multiple spawning in the Molpro quantum chemistry package. *Chemical Physics*, **2008**, 347, 3-16	2.3	174
278	Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer. *Nature Chemistry*, **2014**, 6, 623-8	17.6	157
277	Graphical Processing Units for Quantum Chemistry. *Computing in Science and Engineering*, **2008**, 10, 26-34	1.5	156
276	Excited-State Electronic Structure with Configuration Interaction Singles and Tamm-Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units. *Journal of Chemical Theory and Computation*, **2011**, 7, 1814-1823	6.4	154
275	Conical Intersections in Solution: A QM/MM Study Using Floating Occupation Semiempirical Configuration Interaction Wave Functions. *Journal of Physical Chemistry A*, **2003**, 107, 3822-3830	2.8	153
274	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
273	Inducing and quantifying forbidden reactivity with single-molecule polymer mechanochemistry. *Nature Chemistry*, **2015**, 7, 323-7	17.6	141
272	Ab initio multiple spawning dynamics using multi-state second-order perturbation theory. *Journal of Physical Chemistry A*, **2009**, 113, 13656-62	2.8	138
271	Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics. *Journal of Chemical Physics*, **2014**, 141, 054110	3.9	135
270	Masked cyanoacrylates unveiled by mechanical force. *Journal of the American Chemical Society*, **2010**, 132, 4558-9	16.4	134

269	QTPIE: Charge transfer with polarization current equalization. A fluctuating charge model with correct asymptotics. *Chemical Physics Letters*, **2007**, 438, 315-320	2.5	134
268	Electronic Absorption Spectra from MM and QM/MM Molecular Dynamics: Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein. *Journal of Chemical Theory and Computation*, **2012**, 8, 5092-5106	6.4	133
267	Excited-state dynamics of cytosine reveal multiple intrinsic subpicosecond pathways. *ChemPhysChem*, **2008**, 9, 2486-90	3.2	133
266	Tensor hypercontraction. II. Least-squares renormalization. *Journal of Chemical Physics*, **2012**, 137, 224106	3.9	132
265	The role of intersection topography in bond selectivity of cis-trans photoisomerization. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 1769-73	11.5	125
264	Role of Rydberg states in the photochemical dynamics of ethylene. *Journal of Physical Chemistry A*, **2012**, 116, 2808-18	2.8	119
263	Dynamic Precision for Electron Repulsion Integral Evaluation on Graphical Processing Units (GPUs). *Journal of Chemical Theory and Computation*, **2011**, 7, 949-54	6.4	118
262	Ultrafast X-ray Auger probing of photoexcited molecular dynamics. *Nature Communications*, **2014**, 5, 4235	17.4	117
261	Simulation of the photodynamics of azobenzene on its first excited state: comparison of full multiple spawning and surface hopping treatments. *Journal of Chemical Physics*, **2005**, 123, 234308	3.9	117
260	Imaging CFI conical intersection and photodissociation dynamics with ultrafast electron diffraction. *Science*, **2018**, 361, 64-67	33.3	117
259	Ultrafast internal conversion in ethylene. I. The excited state lifetime. *Journal of Chemical Physics*, **2011**, 134, 244306	3.9	116
258	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
257	Communication: Tensor hypercontraction. III. Least-squares tensor hypercontraction for the determination of correlated wavefunctions. *Journal of Chemical Physics*, **2012**, 137, 221101	3.9	109
256	Variable Electronic Coupling in Phenylacetylene Dendrimers: The Role of Förster, Dexter, and Charge-Transfer Interactions. *Journal of Physical Chemistry A*, **2004**, 108, 671-682	2.8	108
255	Molecular Collision Dynamics on Several Electronic States. *Journal of Physical Chemistry A*, **1997**, 101, 6389-6402	2.8	106
254	Observation of a Zundel-like transition state during proton transfer in aqueous hydroxide solutions. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 15154-9	11.5	105
253	Competitive decay at two- and three-state conical intersections in excited-state intramolecular proton transfer. *Journal of the American Chemical Society*, **2005**, 127, 4560-1	16.4	104
252	Charge Transfer and Polarization in Solvated Proteins from Ab Initio Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2011**, 2, 1789-1793	6.4	103

251	Ab initio excited-state dynamics of the photoactive yellow protein chromophore. *Journal of the American Chemical Society*, **2003**, 125, 12710-1	16.4	103
250	Probing ultrafast □/n□ internal conversion in organic chromophores via K-edge resonant absorption. *Nature Communications*, **2017**, 8, 29	17.4	101
249	The photochemical ring-opening of 1,3-cyclohexadiene imaged by ultrafast electron diffraction. *Nature Chemistry*, **2019**, 11, 504-509	17.6	100
248	Ab initio molecular dynamics of excited-state intramolecular proton transfer using multireference perturbation theory. *Journal of Physical Chemistry A*, **2007**, 111, 11302-10	2.8	99
247	Nonstationary Electronic States and Site-Selective Reactivity. *Journal of Physical Chemistry A*, **1997**, 101, 7702-7710	2.8	97
246	Protonic gating of excited-state twisting and charge localization in GFP chromophores: a mechanistic hypothesis for reversible photoswitching. *Journal of the American Chemical Society*, **2010**, 132, 1192-3	16.4	93
245	Ab initio multiple spawning dynamics of excited butadiene: role of charge transfer. *Journal of Physical Chemistry A*, **2009**, 113, 12815-24	2.8	93
244	Conformationally controlled chemistry: excited-state dynamics dictate ground-state reaction. *Science*, **2007**, 315, 1561-5	33.3	92
243	Ab initio floating occupation molecular orbital-complete active space configuration interaction: an efficient approximation to CASSCF. *Journal of Chemical Physics*, **2010**, 132, 234102	3.9	91
242	Using meta conjugation to enhance charge separation versus charge recombination in phenylacetylene donor-bridge-acceptor complexes. *Journal of the American Chemical Society*, **2005**, 127, 16348-9	16.4	90
241	Meta-conjugation and excited-state coupling in phenylacetylene dendrimers. *Journal of the American Chemical Society*, **2003**, 125, 9288-9	16.4	90
240	Ab initio quantum chemistry for protein structures. *Journal of Physical Chemistry B*, **2012**, 116, 12501-9	3.4	88
239	Quantum Energy Flow and trans-Stilbene Photoisomerization: an Example of a Non-RRKM Reaction□ *Journal of Physical Chemistry A*, **2003**, 107, 10706-10716	2.8	88
238	Ab initio molecular dynamics around a conical intersection: Li(2p) + H2. *Chemical Physics Letters*, **1997**, 272, 139-147	2.5	86
237	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
236	Control of 1,3-cyclohexadiene photoisomerization using light-induced conical intersections. *Journal of Physical Chemistry A*, **2012**, 116, 2758-63	2.8	82
235	The charge transfer problem in density functional theory calculations of aqueously solvated molecules. *Journal of Physical Chemistry B*, **2013**, 117, 12189-201	3.4	82
234	Ab initio molecular dynamics of excited-state intramolecular proton transfer around a three-state conical intersection in malonaldehyde. *Journal of Physical Chemistry A*, **2006**, 110, 618-30	2.8	82

233	Quantum dynamics of the femtosecond photoisomerization of retinal in bacteriorhodopsin. *Faraday Discussions*, **1998**, 447-62; discussion 477-520	3.6	80
232	Classical/quantal method for multistate dynamics: A computational study. *Journal of Chemical Physics*, **1996**, 104, 2847-2856	3.9	80
231	An "optimal" spawning algorithm for adaptive basis set expansion in nonadiabatic dynamics. *Journal of Chemical Physics*, **2009**, 130, 134113	3.9	79
230	Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver. *Physical Review Letters*, **2019**, 122, 230401	7.4	78
229	Multicolor Mechanochromism of a Polymer/Silica Composite with Dual Distinct Mechanophores. *Journal of the American Chemical Society*, **2019**, 141, 1898-1902	16.4	74
228	Ultrafast isomerization initiated by X-ray core ionization. *Nature Communications*, **2015**, 6, 8199	17.4	74
227	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
226	Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways. *Journal of Chemical Theory and Computation*, **2016**, 12, 638-49	6.4	73
225	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
224	Electronic structure of solid 1,3,5-triamino-2,4,6-trinitrobenzene under uniaxial compression: Possible role of pressure-induced metallization in energetic materials. *Physical Review B*, **2003**, 67,	3.3	73
223	Optimization of Conical Intersections with Floating Occupation Semiempirical Configuration Interaction Wave Functions. *Journal of Physical Chemistry A*, **2002**, 106, 4679-4689	2.8	73
222	A remote stereochemical lever arm effect in polymer mechanochemistry. *Journal of the American Chemical Society*, **2014**, 136, 15162-5	16.4	72
221	Revisiting Molecular Dissociation in Density Functional Theory: A Simple Model. *Journal of Chemical Theory and Computation*, **2009**, 5, 770-80	6.4	71
220	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
219	An Ab Initio Exciton Model Including Charge-Transfer Excited States. *Journal of Chemical Theory and Computation*, **2017**, 13, 3493-3504	6.4	66
218	Substituent effects on dynamics at conical intersections: alpha,beta-enones. *Journal of Physical Chemistry A*, **2007**, 111, 11948-60	2.8	66
217	Comparative genomics and site-directed mutagenesis support the existence of only one input channel for protons in the C-family (cbb3 oxidase) of heme-copper oxygen reductases. *Biochemistry* , **2007**, 46, 9963-72	3.2	66
216	Pseudospectral Mo/llerPlesset perturbation theory through third order. *Journal of Chemical Physics*, **1994**, 100, 3631-3638	3.9	64

215	First-principles molecular dynamics on multiple electronic states: A case study of NaI. *Journal of Chemical Physics*, **1996**, 105, 6334-6341	3.9	61
214	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
213	Reactive cross-talk between adjacent tension-trapped transition states. *Journal of the American Chemical Society*, **2011**, 133, 3222-5	16.4	59
212	Ultrafast internal conversion in ethylene. II. Mechanisms and pathways for quenching and hydrogen elimination. *Journal of Chemical Physics*, **2012**, 136, 124317	3.9	59
211	Evolutionary migration of a post-translationally modified active-site residue in the proton-pumping heme-copper oxygen reductases. *Biochemistry*, **2006**, 45, 15405-10	3.2	57
210	A scheme to interpolate potential energy surfaces and derivative coupling vectors without performing a global diabatization. *Journal of Chemical Physics*, **2011**, 135, 224110	3.9	56
209	Excited state direct dynamics of benzene with reparameterized multi-reference semiempirical configuration interaction methods. *Chemical Physics*, **2004**, 304, 133-145	2.3	56
208	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
207	Electronic Absorption and Resonance Raman Spectroscopy from Ab Initio Quantum Molecular Dynamics. *Journal of Physical Chemistry A*, **1999**, 103, 10517-10527	2.8	55
206	Helix switching of a key active-site residue in the cytochrome cbb3 oxidases. *Biochemistry*, **2005**, 44, 10766-75	3.2	54
205	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
204	Electrostatic control of photoisomerization in the photoactive yellow protein chromophore: Ab initio multiple spawning dynamics. *Chemical Physics Letters*, **2008**, 460, 272-277	2.5	53
203	Dynamics of the collisional electron transfer and femtosecond photodissociation of NaI on ab initio electronic energy curves. *Chemical Physics Letters*, **1996**, 259, 252-260	2.5	53
202	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
201	Quartic scaling second-order approximate coupled cluster singles and doubles via tensor hypercontraction: THC-CC2. *Journal of Chemical Physics*, **2013**, 138, 124111	3.9	52
200	Exact tensor hypercontraction: a universal technique for the resolution of matrix elements of local finite-range N-body potentials in many-body quantum problems. *Physical Review Letters*, **2013**, 111, 132505	7.4	51
199	Transient X-ray fragmentation: probing a prototypical photoinduced ring opening. *Physical Review Letters*, **2012**, 108, 253006	7.4	51
198	Time-resolved photoelectron spectroscopy from first principles: excited state dynamics of benzene. *Faraday Discussions*, **2011**, 150, 293-311; discussion 391-418	3.6	51

197	Pseudospectral time-dependent density functional theory. *Journal of Chemical Physics*, **2008**, 128, 104103	3.9	50
196	Local weak pairs spectral and pseudospectral singles and doubles configuration interaction. *Journal of Chemical Physics*, **1996**, 105, 6455-6470	3.9	50
195	Between ethylene and polyenes--the non-adiabatic dynamics of cis-dienes. *Faraday Discussions*, **2012**, 157, 193-212; discussion 243-84	3.6	49
194	Optimization of width parameters for quantum dynamics with frozen Gaussian basis sets. *Chemical Physics*, **2010**, 370, 70-77	2.3	49
193	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
192	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
191	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
190	The cascade unzipping of ladderane reveals dynamic effects in mechanochemistry. *Nature Chemistry*, **2020**, 12, 302-309	17.6	48
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	Tensor hypercontraction equation-of-motion second-order approximate coupled cluster: electronic excitation energies in O(N4) time. *Journal of Physical Chemistry B*, **2013**, 117, 12972-8	3.4	47
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	Multicentered valence electron effective potentials: a solution to the link atom problem for ground and excited electronic states. *Journal of Chemical Physics*, **2006**, 124, 084107	3.9	46
185	Semiclassical Tunneling Rates from Ab Initio Molecular Dynamics. *Journal of Physical Chemistry A*, **1999**, 103, 6055-6059	2.8	44
184	Ab Initio Multiple Spawning Photochemical Dynamics of DMABN Using GPUs. *Journal of Physical Chemistry A*, **2017**, 121, 265-276	2.8	43
183	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
182	Simultaneous observation of nuclear and electronic dynamics by ultrafast electron diffraction. *Science*, **2020**, 368, 885-889	33.3	43
181	A multistate empirical valence bond model for solvation and transport simulations of OH- in aqueous solutions. *Physical Chemistry Chemical Physics*, **2009**, 11, 9420-30	3.6	43
180	Non-adiabatic molecular dynamics: Split-operator multiple spawning with applications to photodissociation. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 941-947		43

179	Modeling mechanophore activation within a viscous rubbery network. *Journal of the Mechanics and Physics of Solids*, **2014**, 63, 141-153	5	42
178	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
177	A charged ring model for classical OH(aq) simulations. *Chemical Physics Letters*, **2007**, 442, 128-133	2.5	42
176	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
175	Modeling mechanophore activation within a crosslinked glassy matrix. *Journal of Applied Physics*, **2013**, 114, 023504	2.5	41
174	Nonlinear dimensionality reduction for nonadiabatic dynamics: the influence of conical intersection topography on population transfer rates. *Journal of Chemical Physics*, **2012**, 137, 22A519	3.9	41
173	Classical Fluctuating Charge Theories: The Maximum Entropy Valence Bond Formalism and Relationships to Previous Models *Journal of Physical Chemistry A*, **2001**, 105, 2842-2850	2.8	41
172	Pseudospectral full configuration interaction. *Journal of Chemical Physics*, **1992**, 97, 1876-1880	3.9	41
171	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. *Journal of Chemical Physics*, **2020**, 152, 224110	3.9	40
170	Disentangling conical intersection and coherent molecular dynamics in methyl bromide with attosecond transient absorption spectroscopy. *Nature Communications*, **2019**, 10, 3133	17.4	40
169	On the extent and connectivity of conical intersection seams and the effects of three-state intersections. *Journal of Physical Chemistry A*, **2008**, 112, 12559-67	2.8	40
168	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
167	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
166	Ab initio molecular dynamics with equation-of-motion coupled-cluster theory: electronic absorption spectrum of ethylene. *Chemical Physics Letters*, **2003**, 375, 299-308	2.5	38
165	Direct imaging of excited electronic states using diffraction techniques: theoretical considerations. *Chemical Physics Letters*, **1996**, 262, 405-414	2.5	38
164	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
163	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
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161	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
160	Exploring the Conical Intersection Seam: The Seam Space Nudged Elastic Band Method. *Journal of Chemical Theory and Computation*, **2013**, 9, 1155-63	6.4	37
159	A unified theoretical framework for fluctuating-charge models in atom-space and in bond-space. *Journal of Chemical Physics*, **2008**, 129, 214113	3.9	37
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157	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
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153	Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations. *Physical Chemistry Chemical Physics*, **2014**, 16, 11770-9	3.6	33
152	Multiple time step integrators in ab initio molecular dynamics. *Journal of Chemical Physics*, **2014**, 140, 084116	3.9	32
151	Ab Initio Reactive Computer Aided Molecular Design. *Accounts of Chemical Research*, **2017**, 50, 652-656	24.3	31
150	Crossing conditions in coupled cluster theory. *Journal of Chemical Physics*, **2017**, 147, 164105	3.9	31
149	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
148	Relation of exact Gaussian basis methods to the dephasing representation: theory and application to time-resolved electronic spectra. *Journal of Chemical Physics*, **2013**, 139, 034112	3.9	30
147	Variational geminal-augmented multireference self-consistent field theory: two-electron systems. *Journal of Chemical Physics*, **2010**, 132, 054103	3.9	29
146	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
145	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
144	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

143	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
142	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
141	Photochemical Dynamics of Ethylene Cation C2H4(.). *Journal of Physical Chemistry Letters*, **2014**, 5, 1467-71	6.4	27
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139	A Continuous Spawning Method for Nonadiabatic Dynamics and Validation for the Zero-Temperature Spin-Boson Problem. *Israel Journal of Chemistry*, **2007**, 47, 75-88	3.4	27
138	Solvation of the Fluoride Anion by Methanol *Journal of Physical Chemistry A*, **2002**, 106, 10015-10021	2.8	27
137	Pseudospectral double excitation configuration interaction. *Journal of Chemical Physics*, **1993**, 98, 7081-7085	3.9	26
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135	A divide and conquer real space finite-element Hartree-Fock method. *Journal of Chemical Physics*, **2010**, 132, 034101	3.9	24
134	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
133	Mixed quantum-classical electrodynamics: Understanding spontaneous decay and zero-point energy. *Physical Review A*, **2018**, 97,	2.6	23
132	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
131	Reduced scaling CASPT2 using supporting subspaces and tensor hyper-contraction. *Journal of Chemical Physics*, **2018**, 149, 044108	3.9	23
130	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
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