Todd J Martinez

List of Publications by Year
in descending order

317 papers	24,527 citations	82 h-index	144 g-index
		5558	9073
353 all docs	353 docs citations	353 times ranked	13678 citing authors

#	Article	IF	Citations
1	Force-induced activation of covalent bonds in mechanoresponsive polymeric materials. Nature, 2009, 459, 68-72.	13.7	1,446
2	Isomerization Through Conical Intersections. Annual Review of Physical Chemistry, 2007, 58, 613-634.	4.8	741
3	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, 2619-2628.	2.3	734
4	Ab Initio Multiple Spawning:â€‰ Photochemistry from First Principles Quantum Molecular Dynamics. Journal of Physical Chemistry A, 2000, 104, 5161-5175.	1.1	717
5	Conical intersections and double excitations in time-dependent density functional theory. Molecular Physics, 2006, 104, 1039-1051.	0.8	557
6	Ab Initio Nonadiabatic Quantum Molecular Dynamics. Chemical Reviews, 2018, 118, 3305-3336.	23.0	459
7	Quantum Chemistry on Graphical Processing Units. 1. Strategies for Two-Electron Integral Evaluation. Journal of Chemical Theory and Computation, 2008, 4, 222-231.	2.3	458
8	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. Journal of Physical Chemistry Letters, 2014, 5, 1885-1891.	2.1	400
9	Multi-Electronic-State Molecular Dynamics:Â A Wave Function Approach with Applications. The Journal of Physical Chemistry, 1996, 100, 7884-7895.	2.9	371
10	Ab Initio Molecular Dynamics and Time-Resolved Photoelectron Spectroscopy of Electronically Excited Uracil and Thymine. Journal of Physical Chemistry A, 2007, 111, 8500-8508.	1.1	355
11	Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field Implementation. Journal of Chemical Theory and Computation, 2009, 5, 1004-1015.	2.3	354
12	Optimizing Conical Intersections without Derivative Coupling Vectors:â€‰ Application to Multistate Multireference Second-Order Perturbation Theory (MS-CASPT2). Journal of Physical Chemistry B, 2008, 112, 405-413.	1.2	340
13	Generating Efficient Quantum Chemistry Codes for Novel Architectures. Journal of Chemical Theory and Computation, 2013, 9, 213-221.	2.3	316
14	Mechanism and Dynamics of Azobenzene Photoisomerization. Journal of the American Chemical Society, 2003, 125, 8098-8099.	6.6	296
15	Discovering chemistry with an ab initio nanoreactor. Nature Chemistry, 2014, 6, 1044-1048.	6.6	286
16	Trapping a Diradical Transition State by Mechanochemical Polymer Extension. Science, 2010, 329, 1057-1060.	6.0	280
17	Ab Initio Quantum Molecular Dynamics. Advances in Chemical Physics, 2002, , 439-512.	0.3	279
18	Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972.	1.2	279

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19	Photodynamics in Complex Environments: Ab Initio Multiple Spawning Quantum Mechanical/Molecular Mechanical Dynamics. Journal of Physical Chemistry B, 2009, 113, 3280-3291.	1.2	259
20	Ab Initio Study of Cisâ^'Trans Photoisomerization in Stilbene and Ethylene. Journal of Physical Chemistry A, 2003, 107, 829-837.	1.1	251
21	Mechanochemical unzipping of insulating polyladderene to semiconducting polyacetylene. Science, 2017, 357, 475-479.	6.0	240
22	Conical intersection dynamics in solution: The chromophore of Green Fluorescent Protein. Faraday Discussions, 2004, 127, 149-163.	1.6	222
23	First Principles Dynamics and Minimum Energy Pathways for Mechanochemical Ring Opening of Cyclobutene. Journal of the American Chemical Society, 2009, 131, 6377-6379.	6.6	219
24	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, 119-126.	7.6	213
25	Tensor hypercontraction density fitting. I. Quartic scaling second- and third-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2012, 137, 044103.	1.2	210
26	Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer. Nature Chemistry, 2014, 6, 623-628.	6.6	198
27	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. Journal of Physical Chemistry B, 2017, 121, 4023-4039.	1.2	192
28	Implementation of ab initio multiple spawning in the Molpro quantum chemistry package. Chemical Physics, 2008, 347, 3-16.	0.9	190
29	Inducing and quantifying forbidden reactivity with single-molecule polymer mechanochemistry. Nature Chemistry, 2015, 7, 323-327.	6.6	182
30	Excited-State Electronic Structure with Configuration Interaction Singles and Tammâ€"Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units. Journal of Chemical Theory and Computation, 2011, 7, 1814-1823.	2.3	180
31	Imaging CF ₃ I conical intersection and photodissociation dynamics with ultrafast electron diffraction. Science, 2018, 361, 64-67.	6.0	170
32	Graphical Processing Units for Quantum Chemistry. Computing in Science and Engineering, 2008, 10, 26-34.	1.2	169
33	Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics. Journal of Chemical Physics, 2014, 141, 054110.	1.2	168
34	QTPIE: Charge transfer with polarization current equalization. A fluctuating charge model with correct asymptotics. Chemical Physics Letters, 2007, 438, 315-320.	1.2	165
35	Conical Intersections in Solution:â€‰ A QM/MM Study Using Floating Occupation Semiempirical Configuration Interaction Wave Functions. Journal of Physical Chemistry A, 2003, 107, 3822-3830.	1.1	162
36	Tensor hypercontraction. II. Least-squares renormalization. Journal of Chemical Physics, 2012, 137, 224106.	1.2	162

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37	Electronic Absorption Spectra from MM and ab Initio QM/MM Molecular Dynamics: Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein. Journal of Chemical Theory and Computation, 2012, 8, 5092-5106.	2.3	158
38	The photochemical ring-opening of 1,3-cyclohexadiene imaged by ultrafast electron diffraction. Nature Chemistry, 2019, 11, 504-509.	6.6	157
39	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.	1.2	150
40	Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver. Physical Review Letters, 2019, 122, 230401.	2.9	150
41	Masked Cyanoacrylates Unveiled by Mechanical Force. Journal of the American Chemical Society, 2010, 132, 4558-4559.	6.6	149
42	Ab Initio Multiple Spawning Dynamics Using Multi-State Second-Order Perturbation Theory. Journal of Physical Chemistry A, 2009, 113, 13656-13662.	1.1	146
43	Probing ultrafast Ï€Ï€*/nÏ€* internal conversion in organic chromophores via K-edge resonant absorption. Nature Communications, 2017, 8, 29.	5.8	144
44	<scp>TeraChem</scp>: A graphical processing unit<scp>â€accelerated</scp> electronic structure package for <scp>largeâ€scale</scp> ab initio molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1494.	6.2	143
45	Excitedâ€State Dynamics of Cytosine Reveal Multiple Intrinsic Subpicosecond Pathways. ChemPhysChem, 2008, 9, 2486-2490.	1.0	142
46	Ultrafast X-ray Auger probing of photoexcited molecular dynamics. Nature Communications, 2014, 5, 4235.	5.8	140
47	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, 1769-1773.	3.3	138
48	Dynamic Precision for Electron Repulsion Integral Evaluation on Graphical Processing Units (GPUs). Journal of Chemical Theory and Computation, 2011, 7, 949-954.	2.3	138
49	Communication: Tensor hypercontraction. III. Least-squares tensor hypercontraction for the determination of correlated wavefunctions. Journal of Chemical Physics, 2012, 137, 221101.	1.2	135
50	Role of Rydberg States in the Photochemical Dynamics of Ethylene. Journal of Physical Chemistry A, 2012, 116, 2808-2818.	1.1	127
51	Ultrafast internal conversion in ethylene. I. The excited state lifetime. Journal of Chemical Physics, 2011, 134, 244306.	1.2	126
52	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.	1.2	121
53	Competitive Decay at Two- and Three-State Conical Intersections in Excited-State Intramolecular Proton Transfer. Journal of the American Chemical Society, 2005, 127, 4560-4561.	6.6	117
54	Molecular Collision Dynamics on Several Electronic States. Journal of Physical Chemistry A, 1997, 101, 6389-6402.	1.1	114

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55	Nonstationary Electronic States and Site-Selective Reactivity. Journal of Physical Chemistry A, 1997, 101, 7702-7710.	1.1	113
56	Charge Transfer and Polarization in Solvated Proteins from Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2011, 2, 1789-1793.	2.1	113
57	Variable Electronic Coupling in Phenylacetylene Dendrimers:â€‰ The Role of FÃ¶rster, Dexter, and Charge-Transfer Interactions. Journal of Physical Chemistry A, 2004, 108, 671-682.	1.1	111
58	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, 15154-15159.	3.3	111
59	Ab Initio Molecular Dynamics of Excited-State Intramolecular Proton Transfer Using Multireference Perturbation Theory. Journal of Physical Chemistry A, 2007, 111, 11302-11310.	1.1	110
60	Ab Initio Multiple Spawning Dynamics of Excited Butadiene: Role of Charge Transfer. Journal of Physical Chemistry A, 2009, 113, 12815-12824.	1.1	109
61	Ab Initio Excited-State Dynamics of the Photoactive Yellow Protein Chromophore. Journal of the American Chemical Society, 2003, 125, 12710-12711.	6.6	108
62	Ab initio floating occupation molecular orbital-complete active space configuration interaction: An efficient approximation to CASSCF. Journal of Chemical Physics, 2010, 132, 234102.	1.2	106
63	Multicolor Mechanochromism of a Polymer/Silica Composite with Dual Distinct Mechanophores. Journal of the American Chemical Society, 2019, 141, 1898-1902.	6.6	105
64	Conformationally Controlled Chemistry: Excited-State Dynamics Dictate Ground-State Reaction. Science, 2007, 315, 1561-1565.	6.0	100
65	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, 1192-1193.	6.6	100
66	Ab initio molecular dynamics around a conical intersection: Li(2p) + H2. Chemical Physics Letters, 1997, 272, 139-147.	1.2	99
67	Ab Initio Quantum Chemistry for Protein Structures. Journal of Physical Chemistry B, 2012, 116, 12501-12509.	1.2	99
68	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.	1.2	98
69	Using Meta Conjugation To Enhance Charge Separation versus Charge Recombination in Phenylacetylene Donorâ^'Bridgeâ^'Acceptor Complexes. Journal of the American Chemical Society, 2005, 127, 16348-16349.	6.6	97
70	Seaming is believing. Nature, 2010, 467, 412-413.	13.7	95
71	Control of 1,3-Cyclohexadiene Photoisomerization Using Light-Induced Conical Intersections. Journal of Physical Chemistry A, 2012, 116, 2758-2763.	1.1	95
72	Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways. Journal of Chemical Theory and Computation, 2016, 12, 638-649.	2.3	95

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73	Quantum Energy Flow andtrans-Stilbene Photoisomerization:Â an Example of a Non-RRKM Reactionâ€. Journal of Physical Chemistry A, 2003, 107, 10706-10716.	1.1	94
74	Meta-Conjugation and Excited-State Coupling in Phenylacetylene Dendrimers. Journal of the American Chemical Society, 2003, 125, 9288-9289.	6.6	93
75	Communication: GAIMSâ€"Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. Journal of Chemical Physics, 2016, 144, 101102.	1.2	93
76	Ab Initio Molecular Dynamics of Excited-State Intramolecular Proton Transfer around a Three-State Conical Intersection in Malonaldehydeâ€. Journal of Physical Chemistry A, 2006, 110, 618-630.	1.1	92
77	The Charge Transfer Problem in Density Functional Theory Calculations of Aqueously Solvated Molecules. Journal of Physical Chemistry B, 2013, 117, 12189-12201.	1.2	92
78	Ultrafast isomerization initiated by X-ray core ionization. Nature Communications, 2015, 6, 8199.	5.8	92
79	Simultaneous observation of nuclear and electronic dynamics by ultrafast electron diffraction. Science, 2020, 368, 885-889.	6.0	92
80	Quantum Chemistry for Solvated Molecules on Graphical Processing Units Using Polarizable Continuum Models. Journal of Chemical Theory and Computation, 2015, 11, 3131-3144.	2.3	91
81	A Remote Stereochemical Lever Arm Effect in Polymer Mechanochemistry. Journal of the American Chemical Society, 2014, 136, 15162-15165.	6.6	89
82	Classical/quantal method for multistate dynamics: A computational study. Journal of Chemical Physics, 1996, 104, 2847-2856.	1.2	87
83	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110.	1.2	87
84	An Ab Initio Exciton Model Including Charge-Transfer Excited States. Journal of Chemical Theory and Computation, 2017, 13, 3493-3504.	2.3	85
85	Revisiting Molecular Dissociation in Density Functional Theory: A Simple Model. Journal of Chemical Theory and Computation, 2009, 5, 770-780.	2.3	84
86	Quantum dynamics of the femtosecond photoisomerization of retinal in bacteriorhodopsin. Faraday Discussions, 1998, 110, 447-462.	1.6	83
87	Ab Initio Nonadiabatic Dynamics of Multichromophore Complexes: A Scalable Graphical-Processing-Unit-Accelerated Exciton Framework. Accounts of Chemical Research, 2014, 47, 2857-2866.	7.6	83
88	An â€œoptimalâ€•spawning algorithm for adaptive basis set expansion in nonadiabatic dynamics. Journal of Chemical Physics, 2009, 130, 134113.	1.2	82
89	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, .	1.1	77
90	The cascade unzipping of ladderane reveals dynamic effects in mechanochemistry. Nature Chemistry, 2020, 12, 302-309.	6.6	76

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91	Optimization of Conical Intersections with Floating Occupation Semiempirical Configuration Interaction Wave Functions. Journal of Physical Chemistry A, 2002, 106, 4679-4689.	1.1	75
92	Substituent Effects on Dynamics at Conical Intersections:â€‰ Î±,Î²-Enones. Journal of Physical Chemistry A, 2007, 111, 11948-11960.	1.1	75
93	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, 5730-5740.	6.6	75
94	Ultrafast internal conversion in ethylene. II. Mechanisms and pathways for quenching and hydrogen elimination. Journal of Chemical Physics, 2012, 136, 124317.	1.2	72
95	Pseudospectral Mo/llerâ€“Plesset perturbation theory through third order. Journal of Chemical Physics, 1994, 100, 3631-3638.	1.2	70
96	Comparative Genomics and Site-Directed Mutagenesis Support the Existence of Only One Input Channel for Protons in the C-Family (cbb₃ Oxidase) of Hemeâ^Copper Oxygen Reductases. Biochemistry, 2007, 46, 9963-9972.	1.2	70
97	Disentangling conical intersection and coherent molecular dynamics in methyl bromide with attosecond transient absorption spectroscopy. Nature Communications, 2019, 10, 3133.	5.8	68
98	Firstâ€principles molecular dynamics on multiple electronic states: A case study of NaI. Journal of Chemical Physics, 1996, 105, 6334-6341.	1.2	66
99	Quartic scaling second-order approximate coupled cluster singles and doubles via tensor hypercontraction: THC-CC2. Journal of Chemical Physics, 2013, 138, 124111.	1.2	66
100	Ab initio multiple cloning simulations of pyrrole photodissociation: TKER spectra and velocity map imaging. Physical Chemistry Chemical Physics, 2015, 17, 3316-3325.	1.3	66
101	Mediation of donorâ€“acceptor distance in an enzymatic methyl transfer reaction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7954-7959.	3.3	65
102	Atomistic non-adiabatic dynamics of the LH2 complex with a GPU-accelerated ab initio exciton model. Physical Chemistry Chemical Physics, 2017, 19, 14924-14936.	1.3	64
103	Evolutionary Migration of a Post-Translationally Modified Active-Site Residue in the Proton-Pumping Heme-Copper Oxygen Reductasesâ€. Biochemistry, 2006, 45, 15405-15410.	1.2	63
104	Pseudospectral time-dependent density functional theory. Journal of Chemical Physics, 2008, 128, 104103.	1.2	63
105	Reactive Cross-Talk between Adjacent Tension-Trapped Transition States. Journal of the American Chemical Society, 2011, 133, 3222-3225.	6.6	63
106	Time-resolved photoelectron spectroscopy from first principles: Excited state dynamics of benzene. Faraday Discussions, 2011, 150, 293.	1.6	61
107	Exact Tensor Hypercontraction: A Universal Technique for the Resolution of Matrix Elements of Local Finite-Range<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>-Body Potentials in Many-Body Quantum Problems. Physical Review Letters, 2013, 111, 132505.	2.9	61
108	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, 1940-1949.	1.2	61

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109	Excited state direct dynamics of benzene with reparameterized multi-reference semiempirical configuration interaction methods. Chemical Physics, 2004, 304, 133-145.	0.9	60
110	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.	1.2	60
111	Dynamics of the collisional electron transfer and femtosecond photodissociation of NaI on ab initio electronic energy curves. Chemical Physics Letters, 1996, 259, 252-260.	1.2	59
112	A scheme to interpolate potential energy surfaces and derivative coupling vectors without performing a global diabatization. Journal of Chemical Physics, 2011, 135, 224110.	1.2	59
113	Electronic Absorption and Resonance Raman Spectroscopy from Ab Initio Quantum Molecular Dynamics. Journal of Physical Chemistry A, 1999, 103, 10517-10527.	1.1	58
114	Communication: Acceleration of coupled cluster singles and doubles via orbital-weighted least-squares tensor hypercontraction. Journal of Chemical Physics, 2014, 140, 181102.	1.2	57
115	Helix Switching of a Key Active-Site Residue in the Cytochromecbb3Oxidasesâ€. Biochemistry, 2005, 44, 10766-10775.	1.2	56
116	Electrostatic control of photoisomerization in the photoactive yellow protein chromophore: Ab initio multiple spawning dynamics. Chemical Physics Letters, 2008, 460, 272-277.	1.2	56
117	Transient X-Ray Fragmentation: Probing a Prototypical Photoinduced Ring Opening. Physical Review Letters, 2012, 108, 253006.	2.9	56
118	Optimization of width parameters for quantum dynamics with frozen Gaussian basis sets. Chemical Physics, 2010, 370, 70-77.	0.9	55
119	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, 2444-2449.	2.1	55
120	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.	2.3	55
121	Between ethylene and polyenes - the non-adiabatic dynamics of cis-dienes. Faraday Discussions, 2012, 157, 193.	1.6	54
122	Tensor Hypercontraction Equation-of-Motion Second-Order Approximate Coupled Cluster: Electronic Excitation Energies in O(N4) Time. Journal of Physical Chemistry B, 2013, 117, 12972-12978.	1.2	54
123	Local weak pairs spectral and pseudospectral singles and doubles configuration interaction. Journal of Chemical Physics, 1996, 105, 6455-6470.	1.2	53
124	Nonlinear dimensionality reduction for nonadiabatic dynamics: The influence of conical intersection topography on population transfer rates. Journal of Chemical Physics, 2012, 137, 22A519.	1.2	53
125	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.	2.3	53
126	Direct observation of ultrafast hydrogen bond strengthening in liquid water. Nature, 2021, 596, 531-535.	13.7	53

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127	Atomic orbital-based SOS-MP2 with tensor hypercontraction. I. GPU-based tensor construction and exploiting sparsity. Journal of Chemical Physics, 2016, 144, 174111.	1.2	52
128	Non-adiabatic molecular dynamics: Split-operator multiple spawning with applications to photodissociation. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 941-947.	1.7	51
129	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.	1.2	51
130	Semiclassical Tunneling Rates from Ab Initio Molecular Dynamics. Journal of Physical Chemistry A, 1999, 103, 6055-6059.	1.1	50
131	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.	1.2	50
132	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.	1.2	50
133	Modeling mechanophore activation within a viscous rubbery network. Journal of the Mechanics and Physics of Solids, 2014, 63, 141-153.	2.3	49
134	Analytical derivatives of the individual state energies in ensemble density functional theory method. I. General formalism. Journal of Chemical Physics, 2017, 147, 034113.	1.2	49
135	Modeling mechanophore activation within a crosslinked glassy matrix. Journal of Applied Physics, 2013, 114, .	1.1	48
136	Ab Initio Multiple Spawning Photochemical Dynamics of DMABN Using GPUs. Journal of Physical Chemistry A, 2017, 121, 265-276.	1.1	48
137	Parallel molecular mechanisms for enzyme temperature adaptation. Science, 2021, 371, .	6.0	48
138	Tensor Hypercontraction Second-Order MÃ¸llerâ€“Plesset Perturbation Theory: Grid Optimization and Reaction Energies. Journal of Chemical Theory and Computation, 2015, 11, 3042-3052.	2.3	47
139	A charged ring model for classical OHâ¯(aq) simulations. Chemical Physics Letters, 2007, 442, 128-133.	1.2	46
140	On the Extent and Connectivity of Conical Intersection Seams and the Effects of Three-State Intersections. Journal of Physical Chemistry A, 2008, 112, 12559-12567.	1.1	46
141	Ab Initio Interactive Molecular Dynamics on Graphical Processing Units (GPUs). Journal of Chemical Theory and Computation, 2015, 11, 4536-4544.	2.3	46
142	Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the nÏ€* and Ï€Ï€* Excited States. Journal of the American Chemical Society, 2020, 142, 20680-20690.	6.6	46
143	Pseudospectral full configuration interaction. Journal of Chemical Physics, 1992, 97, 1876-1880.	1.2	45
144	Ab initio molecular dynamics with equation-of-motion coupled-cluster theory: electronic absorption spectrum of ethylene. Chemical Physics Letters, 2003, 375, 299-308.	1.2	45

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145	A multistate empirical valence bond model for solvation and transport simulations of OHâ˜ in aqueous solutions. Physical Chemistry Chemical Physics, 2009, 11, 9420.	1.3	45
146	Discrete variable representation in electronic structure theory: Quadrature grids for least-squares tensor hypercontraction. Journal of Chemical Physics, 2013, 138, 194107.	1.2	45
147	Direct imaging of excited electronic states using diffraction techniques: theoretical considerations. Chemical Physics Letters, 1996, 262, 405-414.	1.2	44
148	Classical Fluctuating Charge Theories:Â The Maximum Entropy Valence Bond Formalism and Relationships to Previous Modelsâ€. Journal of Physical Chemistry A, 2001, 105, 2842-2850.	1.1	44
149	A unified theoretical framework for fluctuating-charge models in atom-space and in bond-space. Journal of Chemical Physics, 2008, 129, 214113.	1.2	44
150	Exploring the Conical Intersection Seam: The Seam Space Nudged Elastic Band Method. Journal of Chemical Theory and Computation, 2013, 9, 1155-1163.	2.3	44
151	Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units. Journal of Chemical Physics, 2015, 143, 014111.	1.2	44
152	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.	0.6	44
153	Ab Initio Reactive Computer Aided Molecular Design. Accounts of Chemical Research, 2017, 50, 652-656.	7.6	44
154	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.	6.6	43
155	Intermolecular vibrations mediate ultrafast singlet fission. Science Advances, 2020, 6, .	4.7	42
156	Geodesic interpolation for reaction pathways. Journal of Chemical Physics, 2019, 150, 164103.	1.2	41
157	A New Approach to Reactive Potentials with Fluctuating Charges:Â Quadratic Valence-Bond Model. Journal of Physical Chemistry A, 2004, 108, 3076-3084.	1.1	40
158	Crossing conditions in coupled cluster theory. Journal of Chemical Physics, 2017, 147, 164105.	1.2	40
159	Pseudospectral multireference single and double excitation configuration interaction. Journal of Chemical Physics, 1995, 102, 7564-7572.	1.2	39
160	PSEUDOSPECTRAL METHODS APPLIED TO THE ELECTRON CORRELATION PROBLEM. Advanced Series in Physical Chemistry, 1995, , 1132-1165.	1.5	39
161	Rank reduced coupled cluster theory. I. Ground state energies and wavefunctions. Journal of Chemical Physics, 2019, 150, 164118.	1.2	37
162	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.	1.2	35

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163	Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations. Physical Chemistry Chemical Physics, 2014, 16, 11770-11779.	1.3	35
164	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.	1.2	35
165	How Does Peripheral Functionalization of Ruthenium(II)â€"Terpyridine Complexes Affect Spatial Charge Redistribution after Photoexcitation at the Franckâ€"Condon Point?. ChemPhysChem, 2015, 16, 1395-1404.	1.0	34
166	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.	6.6	34
167	Exploiting graphical processing units to enable quantum chemistry calculation of large solvated molecules with conductorâ€like polarizable continuum models. International Journal of Quantum Chemistry, 2019, 119, e25760.	1.0	34
168	Holeâ€"hole Tammâ€"Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. Journal of Chemical Physics, 2020, 153, 024110.	1.2	34
169	Electronic structure software. Journal of Chemical Physics, 2020, 153, 070401.	1.2	34
170	Multiple time step integrators in ab initio molecular dynamics. Journal of Chemical Physics, 2014, 140, 084116.	1.2	33
171	Flyby reaction trajectories: Chemical dynamics under extrinsic force. Science, 2021, 373, 208-212.	6.0	33
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