# Todd J Martinez

List of Publications by Year
in descending order

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|---|---|---|---|
| 317 papers | 24,527 citations | 5569 82 h-index | 9090 144 g-index |
| 353 all docs | 353 docs citations | 353 times ranked | 13678 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Rank-reduced coupled-cluster. III. Tensor hypercontraction of the doubles amplitudes. Journal of Chemical Physics, 2022, 156, 054102. | 1.2 | 15 |
| 2 | Internal conversion of the anionic GFP chromophore: in and out of the I-twisted S<sub>1</sub>/S<sub>0</sub> conical intersection seam. Chemical Science, 2022, 13, 373-385. | 3.7 | 23 |
| 3 | Dissociative electron attachment to 5-bromo-uracil: non-adiabatic dynamics on complex-valued potential energy surfaces. Physical Chemistry Chemical Physics, 2022, 24, 6845-6855. | 1.3 | 3 |
| 4 | Chiral photochemistry of achiral molecules. Nature Communications, 2022, 13, 2091. | 5.8 | 11 |
| 5 | Bringing chemical structures to life with augmented reality, machine learning, and quantum chemistry. Journal of Chemical Physics, 2022, 156, . | 1.2 | 6 |
| 6 | A multi-stage single photochrome system for controlled photoswitching responses. Nature Chemistry, 2022, 14, 942-948. | 6.6 | 18 |
| 7 | Steric and Electronic Origins of Fluorescence in GFP and GFP-like Proteins. Journal of the American Chemical Society, 2022, 144, 12732-12746. | 6.6 | 8 |
| 8 | <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 |
| 9 | Reduced scaling formulation of CASPT2 analytical gradients using the supporting subspace method. Journal of Chemical Physics, 2021, 154, 014103. | 1.2 | 19 |
| 10 | The non-adiabatic nanoreactor: towards the automated discovery of photochemistry. Chemical Science, 2021, 12, 7294-7307. | 3.7 | 31 |
| 11 | USING MACHINE LEARNING TO LEARN CHEMISTRY. , 2021, , . | | 0 |
| 12 | Voice-controlled quantum chemistry. Nature Computational Science, 2021, 1, 42-45. | 3.8 | 8 |
| 13 | Nitromethane Decomposition via Automated Reaction Discovery and an Ab Initio Corrected Kinetic Model. Journal of Physical Chemistry A, 2021, 125, 1447-1460. | 1.1 | 16 |
| 14 | Cover Image, Volume 11, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1523. | 6.2 | 5 |
| 15 | A Tribute to Emily A. Carter. Journal of Physical Chemistry A, 2021, 125, 1669-1670. | 1.1 | 0 |
| 16 | Substituent Effects in Mechanochemical Allowed and Forbidden Cyclobutene Ring-Opening Reactions. Journal of the American Chemical Society, 2021, 143, 3846-3855. | 6.6 | 26 |
| 17 | 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. | 1.2 | 18 |
| 18 | Parallel molecular mechanisms for enzyme temperature adaptation. Science, 2021, 371, . | 6.0 | 48 |

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| 19 | 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. | 1.2 | 8 |
| 20 | A Tribute to Emily A. Carter. Journal of Physical Chemistry C, 2021, 125, 4331-4332. | 1.5 | 0 |
| 21 | Electrostatic Control of Photoisomerization in Channelrhodopsin 2. Journal of the American Chemical Society, 2021, 143, 5425-5437. | 6.6 | 17 |
| 22 | Unmasking the cis-Stilbene Phantom State via Vacuum Ultraviolet Time-Resolved Photoelectron Spectroscopy and Ab Initio Multiple Spawning. Journal of Physical Chemistry Letters, 2021, 12, 6363-6369. | 2.1 | 18 |
| 23 | Understanding the Mechanochemistry of Ladder-Type Cyclobutane Mechanophores by Single Molecule Force Spectroscopy. Journal of the American Chemical Society, 2021, 143, 12328-12334. | 6.6 | 26 |
| 24 | Flyby reaction trajectories: Chemical dynamics under extrinsic force. Science, 2021, 373, 208-212. | 6.0 | 33 |
| 25 | A diagrammatic approach for automatically deriving analytical gradients of tensor hyper-contracted electronic structure methods. Journal of Chemical Physics, 2021, 155, 024108. | 1.2 | 2 |
| 26 | Chemical physics software. Journal of Chemical Physics, 2021, 155, 010401. | 1.2 | 2 |
| 27 | Direct observation of ultrafast hydrogen bond strengthening in liquid water. Nature, 2021, 596, 531-535. | 13.7 | 53 |
| 28 | Observation of conformer-specific photochemical dynamics with MeV ultrafast electron diffraction. , 2021, , . | | 0 |
| 29 | Resolving the ultrafast dynamics of the anionic green fluorescent protein chromophore in water. Chemical Science, 2021, 12, 11347-11363. | 3.7 | 28 |
| 30 | Transient resonant Augerâ€“Meitner spectra of photoexcited thymine. Faraday Discussions, 2021, 228, 555-570. | 1.6 | 11 |
| 31 | ChemPix: automated recognition of hand-drawn hydrocarbon structures using deep learning. Chemical Science, 2021, 12, 10622-10633. | 3.7 | 20 |
| 32 | Conformer-specific photochemistry imaged in real space and time. Science, 2021, 374, 178-182. | 6.0 | 20 |
| 33 | InteraChem: Virtual Reality Visualizer for Reactive Interactive Molecular Dynamics. Journal of Chemical Education, 2021, 98, 3486-3492. | 1.1 | 16 |
| 34 | Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Holeâ€“Hole Tammâ€“Dancoff-Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 7120-7133. | 2.3 | 3 |
| 35 | 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. | 1.2 | 11 |
| 36 | In Silico Discovery of Multistep Chemistry Initiated by a Conical Intersection: The Challenging Case of Donorâ€“Acceptor Stenhouse Adducts. Journal of the American Chemical Society, 2021, 143, 20015-20021. | 6.6 | 18 |

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| 37 | GPU acceleration of rank-reduced coupled-cluster singles and doubles. Journal of Chemical Physics, 2021, 155, 184110. | 1.2 | 6 |
| 38 | Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801. | 1.2 | 15 |
| 39 | 2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401. | 1.2 | 1 |
| 40 | The cascade unzipping of ladderane reveals dynamic effects in mechanochemistry. Nature Chemistry, 2020, 12, 302-309. | 6.6 | 76 |
| 41 | The Mechanics of the Bicycle Pedal Photoisomerization in Crystalline cis,cis-1,4-Diphenyl-1,3-butadiene. Journal of Physical Chemistry A, 2020, 124, 8897-8906. | 1.1 | 6 |
| 42 | Intermolecular vibrations mediate ultrafast singlet fission. Science Advances, 2020, 6, . | 4.7 | 42 |
| 43 | JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402. | 1.2 | 2 |
| 44 | 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 |
| 45 | 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. | 2.3 | 20 |
| 46 | 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 |
| 47 | An ab initio exciton model for singlet fission. Journal of Chemical Physics, 2020, 153, 184116. | 1.2 | 16 |
| 48 | A multilayer multi-configurational approach to efficiently simulate large-scale circuit-based quantum computers on classical machines. Journal of Chemical Physics, 2020, 153, 051101. | 1.2 | 3 |
| 49 | Ab Initio Nonadiabatic Molecular Dynamics with Holeâ€“Hole Tammâ€“Dancoff Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 5499-5511. | 2.3 | 27 |
| 50 | PySpawn: Software for Nonadiabatic Quantum Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 5485-5498. | 2.3 | 10 |
| 51 | Proton Transfer Dynamics in the Aprotic Proton Accepting Solvent 1-Methylimidazole. Journal of Physical Chemistry B, 2020, 124, 7897-7908. | 1.2 | 6 |
| 52 | Putting Photomechanical Switches to Work: An Ab Initio Multiple Spawning Study of Donorâ€“Acceptor Stenhouse Adducts. Journal of Physical Chemistry Letters, 2020, 11, 7901-7907. | 2.1 | 21 |
| 53 | Electronic structure software. Journal of Chemical Physics, 2020, 153, 070401. | 1.2 | 34 |
| 54 | Fast transformations between configuration state function and Slater determinant bases for direct configuration interaction. Journal of Chemical Physics, 2020, 152, 164111. | 1.2 | 11 |

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| 55 | Strictly non-adiabatic quantum control of the acetylene dication using an infrared field. Journal of Chemical Physics, 2020, 152, 184302. | 1.2 | 1 |
| 56 | Nonadiabatic Dynamics of Photoexcited cis-Stilbene Using Ab Initio Multiple Spawning. Journal of Physical Chemistry B, 2020, 124, 5476-5487. | 1.2 | 24 |
| 57 | Simultaneous observation of nuclear and electronic dynamics by ultrafast electron diffraction. Science, 2020, 368, 885-889. | 6.0 | 92 |
| 58 | TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110. | 1.2 | 87 |
| 59 | Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures. Journal of Chemical Theory and Computation, 2020, 16, 4021-4028. | 2.3 | 22 |
| 60 | Reduced scaling extended multi-state CASPT2 (XMS-CASPT2) using supporting subspaces and tensor hyper-contraction. Journal of Chemical Physics, 2020, 152, 234113. | 1.2 | 17 |
| 61 | Matter-wave interference of a native polypeptide. Nature Communications, 2020, 11, 1447. | 5.8 | 23 |
| 62 | Strong, Nonresonant Radiation Enhances Cisâ€“Trans Photoisomerization of Stilbene in Solution. Journal of Physical Chemistry A, 2020, 124, 5999-6008. | 1.1 | 7 |
| 63 | SSAIMSâ€”Stochastic-Selection Ab Initio Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry A, 2020, 124, 6133-6143. | 1.1 | 13 |
| 64 | 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. | 2.5 | 21 |
| 65 | Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy. Chemical Science, 2020, 11, 4180-4193. | 3.7 | 29 |
| 66 | Reaction Dynamics of Cyanohydrins with Hydrosulfide in Water. Journal of Physical Chemistry A, 2019, 123, 7210-7217. | 1.1 | 4 |
| 67 | On combining the conductor-like screening model and optimally tuned range-separated hybrid density functionals. Journal of Chemical Physics, 2019, 150, 174117. | 1.2 | 9 |
| 68 | Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2019, 123, 6897-6903. | 1.1 | 29 |
| 69 | Disentangling conical intersection and coherent molecular dynamics in methyl bromide with attosecond transient absorption spectroscopy. Nature Communications, 2019, 10, 3133. | 5.8 | 68 |
| 70 | Photo-protection/photo-damage in natural systems: general discussion. Faraday Discussions, 2019, 216, 538-563. | 1.6 | 4 |
| 71 | Photovoltaics and bio-inspired light harvesting: general discussion. Faraday Discussions, 2019, 216, 269-300. | 1.6 | 0 |
| 72 | 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 |

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| 73 | Diffractive imaging of dissociation and ground-state dynamics in a complex molecule. Physical Review A, 2019, 100, . | 1.0 | 21 |
| 74 | Imaging the ring opening reaction of 1,3-cyclohexadiene with MeV ultrafast electron diffraction. EPJ Web of Conferences, 2019, 205, 07006. | 0.1 | 0 |
| 75 | Computational Discovery of the Origins of Life. ACS Central Science, 2019, 5, 1493-1495. | 5.3 | 19 |
| 76 | Sub-Femtosecond Stark Control of Molecular Photoexcitation with Near Single-Cycle Pulses. Journal of Physical Chemistry Letters, 2019, 10, 742-747. | 2.1 | 10 |
| 77 | Ab Initio Computation of Rotationally-Averaged Pumpâ€“Probe X-ray and Electron Diffraction Signals. Journal of Chemical Theory and Computation, 2019, 15, 1523-1537. | 2.3 | 24 |
| 78 | Multicolor Mechanochromism of a Polymer/Silica Composite with Dual Distinct Mechanophores. Journal of the American Chemical Society, 2019, 141, 1898-1902. | 6.6 | 105 |
| 79 | Perturbation of Short Hydrogen Bonds in Photoactive Yellow Protein via Noncanonical Amino Acid Incorporation. Journal of Physical Chemistry B, 2019, 123, 4844-4849. | 1.2 | 12 |
| 80 | Electrostatic Influence on Photoisomerization in Bacteriorhodopsin and Halorhodopsin. Journal of Physical Chemistry B, 2019, 123, 4850-4857. | 1.2 | 4 |
| 81 | Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver. Physical Review Letters, 2019, 122, 230401. | 2.9 | 150 |
| 82 | Nonadiabatic Photodynamics of Retinal Protonated Schiff Base in Channelrhodopsin 2. Journal of Physical Chemistry Letters, 2019, 10, 2862-2868. | 2.1 | 25 |
| 83 | Rank reduced coupled cluster theory. I. Ground state energies and wavefunctions. Journal of Chemical Physics, 2019, 150, 164118. | 1.2 | 37 |
| 84 | The photochemical ring-opening of 1,3-cyclohexadiene imaged by ultrafast electron diffraction. Nature Chemistry, 2019, 11, 504-509. | 6.6 | 157 |
| 85 | Geodesic interpolation for reaction pathways. Journal of Chemical Physics, 2019, 150, 164103. | 1.2 | 41 |
| 86 | 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. | 1.1 | 17 |
| 87 | Rank reduced coupled cluster theory. II. Equation-of-motion coupled-cluster singles and doubles. Journal of Chemical Physics, 2019, 151, 164121. | 1.2 | 13 |
| 88 | 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 |
| 89 | Ab Initio Nonadiabatic Quantum Molecular Dynamics. Chemical Reviews, 2018, 118, 3305-3336. | 23.0 | 459 |
| 90 | 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 |

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| 91 | Large-Scale Functional Group Symmetry-Adapted Perturbation Theory on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 1737-1753. | 2.3 | 19 |
| 92 | 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 |
| 93 | A program for automatically predicting supramolecular aggregates and its application to urea and porphin. Journal of Computational Chemistry, 2018, 39, 763-772. | 1.5 | 9 |
| 94 | 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 |
| 95 | Mixed quantum-classical electrodynamics: Understanding spontaneous decay and zero-point energy. Physical Review A, 2018, 97, . | 1.0 | 27 |
| 96 | 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. | 1.1 | 10 |
| 97 | Photoannealing of Merocyanine Aggregates. Journal of Physical Chemistry A, 2018, 122, 9821-9832. | 1.1 | 8 |
| 98 | Imaging CF <sub>3</sub> I conical intersection and photodissociation dynamics with ultrafast electron diffraction. Science, 2018, 361, 64-67. | 6.0 | 170 |
| 99 | Reduced scaling CASPT2 using supporting subspaces and tensor hyper-contraction. Journal of Chemical Physics, 2018, 149, 044108. | 1.2 | 31 |
| 100 | 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 |
| 101 | Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. Journal of Chemical Theory and Computation, 2018, 14, 4139-4150. | 2.3 | 23 |
| 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 | 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 |
| 104 | An Ab Initio Exciton Model Including Charge-Transfer Excited States. Journal of Chemical Theory and Computation, 2017, 13, 3493-3504. | 2.3 | 85 |
| 105 | Atomic orbital-based SOS-MP2 with tensor hypercontraction. II. Local tensor hypercontraction. Journal of Chemical Physics, 2017, 146, 034104. | 1.2 | 29 |
| 106 | Î±-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. | 2.1 | 31 |
| 107 | Probing ultrafast ÏŒ€*/nÏ€* internal conversion in organic chromophores via K-edge resonant absorption. Nature Communications, 2017, 8, 29. | 5.8 | 144 |
| 108 | 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 |

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| 109 | Ab Initio Reactive Computer Aided Molecular Design. Accounts of Chemical Research, 2017, 50, 652-656. | 7.6 | 44 |
| 110 | Ab Initio Multiple Spawning Photochemical Dynamics of DMABN Using GPUs. Journal of Physical Chemistry A, 2017, 121, 265-276. | 1.1 | 48 |
| 111 | Absorption and Fluorescence Features of an Amphiphilic meso-Pyrimidinylcorrole: Experimental Study and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2017, 121, 8614-8624. | 1.1 | 14 |
| 112 | Pomeranzâ€“Fritsch Synthesis of Isoquinoline: Gas-Phase Collisional Activation Opens Additional Reaction Pathways. Journal of the American Chemical Society, 2017, 139, 14352-14355. | 6.6 | 15 |
| 113 | Ultrafast isomerization in acetylene dication after carbon K-shell ionization. Nature Communications, 2017, 8, 453. | 5.8 | 31 |
| 114 | Analytical gradients for tensor hyper-contracted MP2 and SOS-MP2 on graphical processing units. Journal of Chemical Physics, 2017, 147, 161723. | 1.2 | 21 |
| 115 | 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 |
| 116 | The Spin-Flip Variant of the Algebraic-Diagrammatic Construction Yields the Correct Topology of S<sub>1</sub>/S<sub>0</sub> Conical Intersections. Journal of Chemical Theory and Computation, 2017, 13, 4436-4441. | 2.3 | 28 |
| 117 | Mechanochemical unzipping of insulating polyladderene to semiconducting polyacetylene. Science, 2017, 357, 475-479. | 6.0 | 240 |
| 118 | Description of ground and excited electronic states by ensemble density functional method with extended active space. Journal of Chemical Physics, 2017, 147, 064104. | 1.2 | 27 |
| 119 | Crossing conditions in coupled cluster theory. Journal of Chemical Physics, 2017, 147, 164105. | 1.2 | 40 |
| 120 | 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. | 2.3 | 32 |
| 121 | Probing molecular photoinduced dynamics by ultrafast soft x-rays. , 2017, , . | | 1 |
| 122 | Observing Femtosecond Fragmentation Using Ultrafast X-ray-Induced Auger Spectra. Applied Sciences (Switzerland), 2017, 7, 681. | 1.3 | 19 |
| 123 | Adapting DFT+U for the Chemically Motivated Correction of Minimal Basis Set Incompleteness. Journal of Physical Chemistry A, 2016, 120, 5939-5949. | 1.1 | 19 |
| 124 | Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. Journal of Chemical Physics, 2016, 145, 244104. | 1.2 | 23 |
| 125 | Communication: A difference density picture for the self-consistent field ansatz. Journal of Chemical Physics, 2016, 144, 131101. | 1.2 | 6 |
| 126 | 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 |

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| 127 | Comment on â€œPositive semidefinite tensor factorizations of the two-electron integral matrix for low-scalingab initioelectronic structureâ€•[J. Chem. Phys. 143, 064103 (2015)]. Journal of Chemical Physics, 2016, 145, 027101. | 1.2 | 1 |
| 128 | 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 |
| 129 | Communication: XFAIMSâ€”eXternal Field Ab Initio Multiple Spawning for electron-nuclear dynamics triggered by short laser pulses. Journal of Chemical Physics, 2016, 145, 191104. | 1.2 | 31 |
| 130 | Rich Athermal Groundâ€State Chemistry Triggered by Dynamics through a Conical Intersection. Angewandte Chemie, 2016, 128, 15217-15220. | 1.6 | 12 |
| 131 | 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 |
| 132 | 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. | 1.5 | 15 |
| 133 | Toward fully quantum modelling of ultrafast photodissociation imaging experiments. Treating tunnelling in the ab initio multiple cloning approach. Faraday Discussions, 2016, 194, 81-94. | 1.6 | 26 |
| 134 | Pressure-Induced Neutral-to-Ionic Transition in an Amorphous Organic Material. Chemistry of Materials, 2016, 28, 6446-6449. | 3.2 | 4 |
| 135 | Rich Athermal Groundâ€State Chemistry Triggered by Dynamics through a Conical Intersection. Angewandte Chemie - International Edition, 2016, 55, 14993-14996. | 7.2 | 29 |
| 136 | â€œBalancingâ€•the Block Davidsonâ€“Liu Algorithm. Journal of Chemical Theory and Computation, 2016, 12, 3003-3007. | 2.3 | 23 |
| 137 | GPU-Accelerated State-Averaged Complete Active Space Self-Consistent Field Interfaced with Ab Initio Multiple Spawning Unravels the Photodynamics of Provitamin D<sub>3</sub>. Journal of Physical Chemistry Letters, 2016, 7, 2444-2449. | 2.1 | 55 |
| 138 | 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 |
| 139 | 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 |
| 140 | Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. Physical Chemistry Chemical Physics, 2016, 18, 21040-21050. | 1.3 | 22 |
| 141 | Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways. Journal of Chemical Theory and Computation, 2016, 12, 638-649. | 2.3 | 95 |
| 142 | Transient NEXAFS Spectroscopy at the Oxygen Edge: Pinning Down Ï€Ï€*/nÏ€* Internal Conversion. , 2016, , . | | 1 |
| 143 | Evidence of Hydrogen Migration rather than Isomerization in the Acetylene Dication. , 2016, , . | | 0 |
| 144 | Efficient implementation of effective core potential integrals and gradients on graphical processing units. Journal of Chemical Physics, 2015, 143, 014114. | 1.2 | 17 |

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| 145 | 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 |
| 146 | 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 |
| 147 | Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. Journal of Chemical Physics, 2015, 143, 102601. | 1.2 | 10 |
| 148 | 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 |
| 149 | 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, 6875-6883. | 1.1 | 19 |
| 150 | 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 |
| 151 | Direct QM/MM Excited-State Dynamics of Retinal Protonated Schiff Base in Isolation and Methanol Solution. Journal of Physical Chemistry B, 2015, 119, 704-714. | 1.2 | 32 |
| 152 | Inducing and quantifying forbidden reactivity with single-molecule polymer mechanochemistry. Nature Chemistry, 2015, 7, 323-327. | 6.6 | 182 |
| 153 | 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 |
| 154 | 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 |
| 155 | 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 |
| 156 | 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, 14096-14106. | 1.3 | 31 |
| 157 | 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 |
| 158 | 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 |
| 159 | Ab Initio Interactive Molecular Dynamics on Graphical Processing Units (GPUs). Journal of Chemical Theory and Computation, 2015, 11, 4536-4544. | 2.3 | 46 |
| 160 | Catch and Release: Orbital Symmetry Guided Reaction Dynamics from a Freed â€œTension Trapped Transition Stateâ€. Journal of Organic Chemistry, 2015, 80, 11773-11778. | 1.7 | 14 |
| 161 | Ultrafast isomerization initiated by X-ray core ionization. Nature Communications, 2015, 6, 8199. | 5.8 | 92 |
| 162 | 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 |

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