Michael Filatov

List of Publications by Year
in descending order

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88	4,108	81889	118840
papers	citations	39 h-index	62 g-index

90	90	90	2486
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm. Chemistry - A European Journal, 1998, 4, 193-199.	3.3	346
2	A spin-restricted ensemble-referenced Kohnâ€“Sham method and its application to diradicaloid situations. Chemical Physics Letters, 1999, 304, 429-437.	2.6	217
3	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. Journal of Chemical Theory and Computation, 2014, 10, 3074-3084.	5.3	161
4	Theoretical Investigation of Two-State-Reactivity Pathways of Hâˆ’H Activation by FeO+:Â Additionâˆ’Elimination, â€œReboundâ€, and Oxene-Insertion Mechanisms. Journal of Physical Chemistry A, 1998, 102, 3835-3846.	2.5	145
5	Spin-restricted density functional approach to the open-shell problem. Chemical Physics Letters, 1998, 288, 689-697.	2.6	143
6	Surface Hopping Excited-State Dynamics Study of the Photoisomerization of a Light-Driven Fluorene Molecular Rotary Motor. Journal of Chemical Theory and Computation, 2011, 7, 2189-2199.	5.3	134
7	Application of spin-restricted open-shell Kohnâ€“Sham method to atomic and molecular multiplet states. Journal of Chemical Physics, 1999, 110, 116-125.	3.0	122
8	Restricted Ensemble-Referenced Kohnâˆ’Sham versus Broken Symmetry Approaches in Density Functional Theory:â€‰ Magnetic Coupling in Cu Binuclear Complexes. Journal of Chemical Theory and Computation, 2007, 3, 764-774.	5.3	113
9	Implicit and Explicit Coverage of Multi-reference Effects by Density Functional Theory. International Journal of Molecular Sciences, 2002, 3, 604-638.	4.1	111
10	Spinâ€restricted ensembleâ€referenced Kohnâ€“Sham method: basic principles and application to strongly correlated ground and excited states of molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 146-167.	14.6	111
11	Understanding the Dynamics Behind the Photoisomerization of a Light-Driven Fluorene Molecular Rotary Motor. Journal of Physical Chemistry A, 2010, 114, 5058-5067.	2.5	96
12	Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model. Journal of Chemical Theory and Computation, 2013, 9, 3917-3932.	5.3	91
13	On the â€œReboundâ€•Mechanism of Alkane Hydroxylation by Cytochrome P450: Electronic Structure of the Intermediate and the Electron Transfer Character in the Rebound Step. Angewandte Chemie - International Edition, 1999, 38, 3510-3512.	13.8	86
14	Assessment of approximate computational methods for conical intersections and branching plane vectors in organic molecules. Journal of Chemical Physics, 2014, 141, 124122.	3.0	71
15	Designing Conical Intersections for Light-Driven Single Molecule Rotary Motors: From Precessional to Axial Motion. Journal of Organic Chemistry, 2014, 79, 3587-3600.	3.2	67
16	Computational Design of a Family of Light-Driven Rotary Molecular Motors with Improved Quantum Efficiency. Journal of Physical Chemistry Letters, 2016, 7, 105-110.	4.6	67
17	m-Benzyne and bicyclo[3.1.0]hexatriene â€“ which isomer is more stable? â€“ a quantum chemical investigation. Chemical Physics Letters, 2001, 348, 115-125.	2.6	64
18	On the calculation of MÃ¶ssbauer isomer shift. Journal of Chemical Physics, 2007, 127, 084101.	3.0	63

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19	Assessment of Density Functional Methods for Obtaining Geometries at Conical Intersections in Organic Molecules. Journal of Chemical Theory and Computation, 2013, 9, 4526-4541.	5.3	63
20	Tetramethyleneethane (TME) Diradical:Â Experiment and Density Functional Theory Reach an Agreement. Journal of Physical Chemistry A, 1999, 103, 8885-8889.	2.5	61
21	First principles calculation of MÃ¶ssbauer isomer shift. Coordination Chemistry Reviews, 2009, 253, 594-605.	18.8	59
22	Eliminating spin-contamination of spin-flip time dependent density functional theory within linear response formalism by the use of zeroth-order mixed-reference (MR) reduced density matrix. Journal of Chemical Physics, 2018, 149, 104101.	3.0	59
23	Excitation Energies from Spin-Restricted Ensemble-Referenced Kohnâ^'Sham Method: A State-Average Approach. Journal of Physical Chemistry A, 2008, 112, 12980-12988.	2.5	55
24	On convergence of the normalized elimination of the small component (NESC) method. Theoretical Chemistry Accounts, 2007, 117, 333-338.	1.4	52
25	Spin-orbit coupling calculations with the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2013, 139, 014106.	3.0	51
26	Analytical derivatives of the individual state energies in ensemble density functional theory method. I. General formalism. Journal of Chemical Physics, 2017, 147, 034113.	3.0	49
27	Fulgides as Light-Driven Molecular Rotary Motors: Computational Design of a Prototype Compound. Journal of Physical Chemistry Letters, 2018, 9, 4995-5001.	4.6	48
28	Diracâ€exact relativistic methods: the normalized elimination of the small component method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 436-467.	14.6	45
29	Comment on â€œQuasirelativistic theory equivalent to fully relativistic theoryâ€•[J. Chem. Phys. 123, 241102 (2005)]. Journal of Chemical Physics, 2006, 125, 107101.	3.0	44
30	Development, Implementation, and Application of an Analytic Second Derivative Formalism for the Normalized Elimination of the Small Component Method. Journal of Chemical Theory and Computation, 2012, 8, 2617-2629.	5.3	44
31	Design, Synthesis, and Dynamics of a Green Fluorescent Protein Fluorophore Mimic with an Ultrafast Switching Function. Journal of the American Chemical Society, 2016, 138, 9807-9825.	13.7	44
32	Ensemble DFT Approach to Excited States of Strongly Correlated Molecular Systems. Topics in Current Chemistry, 2015, 368, 97-124.	4.0	42
33	An improved algorithm for the normalized elimination of the small-component method. Theoretical Chemistry Accounts, 2011, 130, 633-644.	1.4	41
34	DFT Approach to the Calculation of MÃ¶ssbauer Isomer Shifts. Journal of Chemical Theory and Computation, 2008, 4, 278-285.	5.3	40
35	Analytic Calculation of Isotropic Hyperfine Structure Constants Using the Normalized Elimination of the Small Component Formalism. Journal of Physical Chemistry A, 2012, 116, 3481-3486.	2.5	40
36	Analytic Calculation of Contact Densities and MÃ¶ssbauer Isomer Shifts Using the Normalized Elimination of the Small-Component Formalism. Journal of Chemical Theory and Computation, 2012, 8, 875-882.	5.3	40

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37	Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. Journal of Chemical Physics, 2015, 142, 184104.	3.0	40
38	Assessment of density functional theory based Î”SCF (self-consistent field) and linear response methods for longest wavelength excited states of extended Ï€-conjugated molecular systems. Journal of Chemical Physics, 2014, 141, 024112.	3.0	39
39	Analytical energy gradient for the two-component normalized elimination of the small component method. Journal of Chemical Physics, 2015, 142, 214106.	3.0	39
40	Relief of excited-state antiaromaticity enables the smallest red emitter. Nature Communications, 2021, 12, 5409.	12.8	38
41	Calculation of spin-densities within the context of density functional theory. The crucial role of the correlation functional. Journal of Chemical Physics, 2005, 123, 124101.	3.0	37
42	Description of Conical Intersections with Density Functional Methods. Topics in Current Chemistry, 2015, 368, 445-476.	4.0	37
43	Alkane Hydroxylation by Cytochrome P450: Is Kinetic Isotope Effect a Reliable Probe of Transition State Structure?. European Journal of Inorganic Chemistry, 2000, 2000, 2455-2458.	2.0	35
44	Conical Intersections in Organic Molecules: Benchmarking Mixed-Reference Spinâ€“Flip Time-Dependent DFT (MRSF-TD-DFT) vs Spinâ€“Flip TD-DFT. Journal of Physical Chemistry A, 2019, 123, 6455-6462.	2.5	35
45	Calibration of 57Fe isomer shift from ab initio calculations: can theory and experiment reach an agreement?. Physical Chemistry Chemical Physics, 2010, 12, 2758.	2.8	34
46	Design and photoisomerization dynamics of a new family of synthetic 2-stroke light driven molecular rotary motors. Chemical Communications, 2019, 55, 5247-5250.	4.1	34
47	Non-adiabatic dynamics of ring opening in cyclohexa-1,3-diene described by an ensemble density-functional theory method. Molecular Physics, 2019, 117, 1128-1141.	1.7	33
48	Direct Nonadiabatic Dynamics by Mixed Quantum-Classical Formalism Connected with Ensemble Density Functional Theory Method: Application to trans-Penta-2,4-dieniminium Cation. Journal of Chemical Theory and Computation, 2018, 14, 4499-4512.	5.3	30
49	Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids. Journal of Chemical Theory and Computation, 2021, 17, 848-859.	5.3	29
50	Description of ground and excited electronic states by ensemble density functional method with extended active space. Journal of Chemical Physics, 2017, 147, 064104.	3.0	27
51	Performance Analysis and Optimization of Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) for Vertical Excitation Energies and Singletâ€“Triplet Energy Gaps. Journal of Physical Chemistry A, 2019, 123, 7991-8000.	2.5	27
52	Relativistically corrected electric field gradients calculated with the normalized elimination of the small component formalism. Journal of Chemical Physics, 2012, 137, 054113.	3.0	26
53	Bondpseudorotation, Jahnâ€Teller, and pseudoâ€Jahnâ€Teller effects in the cyclopentadienyl cation and its pentahalogeno derivatives. International Journal of Quantum Chemistry, 2012, 112, 3277-3288.	2.0	25
54	Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. Journal of Physical Chemistry Letters, 2021, 12, 4339-4346.	4.6	24

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55	Calculation of response properties with the normalized elimination of the small component method. International Journal of Quantum Chemistry, 2014, 114, 993-1005.	2.0	23
56	Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. Journal of Chemical Physics, 2016, 145, 244104.	3.0	23
57	Theoretical modelling of the dynamics of primary photoprocess of cyclopropanone. Physical Chemistry Chemical Physics, 2019, 21, 2489-2498.	2.8	23
58	Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. Physical Chemistry Chemical Physics, 2016, 18, 21040-21050.	2.8	22
59	Optimization of Three State Conical Intersections by Adaptive Penalty Function Algorithm in Connection with the Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory Method (MRSF-TDDFT). Journal of Physical Chemistry A, 2021, 125, 1994-2006.	2.5	21
60	Calibration of S119n isomer shift usingab initiowave function methods. Journal of Chemical Physics, 2009, 130, 124121.	3.0	19
61	Nextâ€generation quantum theory of atoms in molecules for the ground and excited states of fulvene. International Journal of Quantum Chemistry, 2018, 118, e25768.	2.0	18
62	Nextâ€generation quantum theory of atoms in molecules for the ground and excited state of the ringâ€opening of cyclohexadiene. International Journal of Quantum Chemistry, 2019, 119, e25862.	2.0	18
63	Communication: On the isotope anomaly of nuclear quadrupole coupling in molecules. Journal of Chemical Physics, 2012, 137, 131102.	3.0	16
64	On multiferroicity of TTF-CA molecular crystal. Physical Chemistry Chemical Physics, 2011, 13, 144-148.	2.8	15
65	A QTAIM and stress tensor investigation of the torsion path of a light-driven fluorene molecular rotary motor. Journal of Computational Chemistry, 2016, 37, 2588-2596.	3.3	15
66	Fast and Accurate Computation of Nonadiabatic Coupling Matrix Elements Using the Truncated Leibniz Formula and Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory. Journal of Physical Chemistry Letters, 2021, 12, 4722-4728.	4.6	15
67	Description of electron transfer in the ground and excited states of organic donorâ€“acceptor systems by single-reference and multi-reference density functional methods. Journal of Chemical Physics, 2014, 141, 124123.	3.0	14
68	Internal Conversion between Bright (1¹B_u⁺) and Dark (2¹A_g^{â€“}) States in s-trans-Butadiene and s-trans-Hexatriene. Journal of Physical Chemistry Letters, 2021, 12, 9720-9729.	4.6	14
69	Nextâ€generation quantum theory of atoms in molecules for the photochemical ringâ€opening reactions of oxirane. International Journal of Quantum Chemistry, 2019, 119, e25957.	2.0	12
70	Nextâ€generation quantum theory of atoms in molecules for the S₁/S₀ conical intersections in dynamics trajectories of a lightâ€driven rotary molecular motor. International Journal of Quantum Chemistry, 2020, 120, e26062.	2.0	12
71	How Beneficial Is the Explicit Account of Doubly-Excited Configurations in Linear Response Theory?. Journal of Chemical Theory and Computation, 2021, 17, 975-984.	5.3	12
72	Exploring Dysonâ€™s Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. Journal of Physical Chemistry Letters, 2021, 12, 9963-9972.	4.6	11

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73	Understanding the dynamics behind photoisomerization of lightâ€driven molecular rotary motors. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 427-437.	14.6	10
74	Calculation of contact densities and MÃ¶ssbauer isomer shifts utilising the Dirac-exact two-component normalised elimination of the small component (2c-NESC) method. Molecular Physics, 2019, 117, 1164-1171.	1.7	10
75	Formulation and Implementation of the Spin-Restricted Ensemble-Referenced Kohnâ€“Sham Method in the Context of the Density Functional Tight Binding Approach. Journal of Chemical Theory and Computation, 2019, 15, 3021-3032.	5.3	10
76	Computation of Molecular Electron Affinities Using an Ensemble Density Functional Theory Method. Journal of Physical Chemistry A, 2020, 124, 7795-7804.	2.5	10
77	Antiferromagnetic interactions in the quarter-filled organic conductor (EDO-TTF)2PF6. Physical Chemistry Chemical Physics, 2011, 13, 12328.	2.8	9
78	A 3â€Ð bonding perspective of the factors influencing the relative stability of the S1/S0conical intersections of the pentaâ€2,4â€dieniminium cation (PSB3). International Journal of Quantum Chemistry, 2019, 119, e25903.	2.0	9
79	Structural or population dynamics: what is revealed by the time-resolved photoelectron spectroscopy of 1,3-cyclohexadiene? A study with an ensemble density functional theory method. Physical Chemistry Chemical Physics, 2020, 22, 17567-17573.	2.8	9
80	Computation of Molecular Ionization Energies Using an Ensemble Density Functional Theory Method. Journal of Chemical Theory and Computation, 2020, 16, 4489-4504.	5.3	8
81	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.	3.0	8
82	Recent advances in ensemble density functional theory and linear response theory for strong correlation. Bulletin of the Korean Chemical Society, 2022, 43, 17-34.	1.9	8
83	MÃ¶ssbauer isomer shifts and effective contact densities obtained by the exact two-component (X2C) relativistic method and its local variants. Physical Chemistry Chemical Physics, 2020, 22, 26776-26786.	2.8	7
84	Description of Sudden Polarization in the Excited Electronic States with an Ensemble Density Functional Theory Method. Journal of Chemical Theory and Computation, 2021, 17, 5123-5139.	5.3	7
85	Accelerated Deep Learning Dynamics for Atomic Layer Deposition of Al(Me)₃ and Water on OH/Si(111). ACS Applied Materials & Interfaces, 2022, 14, 26116-26127.	8.0	5
86	Signatures of Conical Intersection Dynamics in the Time-Resolved Photoelectron Spectrum of Furan: Theoretical Modeling with an Ensemble Density Functional Theory Method. International Journal of Molecular Sciences, 2021, 22, 4276.	4.1	4
87	Manifestations of strong electron correlation in polyacene: Fundamental gap, density of states, and photoconductivity. Carbon Trends, 2022, 7, 100146.	3.0	3
88	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm. , 0, .		2