Michael Filatov

List of Publications by Year in Descending Order

87 papers	3,282 citations	33 h-index	55 g-index
90 ext. papers	3,683 ext. citations	4.8 avg, IF	5.85 L-index

#	Paper	IF	Citations
87	Manifestations of strong electron correlation in polyacene: Fundamental gap, density of states, and photoconductivity. *Carbon Trends*, **2022**, 7, 100146	0	0
86	Exploring Dyson's Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. *Journal of Physical Chemistry Letters*, **2021**, 12, 9963-9972	6.4	2
85	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	2.8	6
84	Analytical derivatives of the individual state energies in ensemble density functional theory. II. Implementation on graphical processing units (GPUs). *Journal of Chemical Physics*, **2021**, 154, 104108	3.9	4
83	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,	6.3	1
82	Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. *Journal of Physical Chemistry Letters*, **2021**, 12, 4339-4346	6.4	9
81	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	6.4	6
80	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	6.4	8
79	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	6.4	2
78	Internal Conversion between Bright (1) and Dark (2) States in s--Butadiene and s--Hexatriene. *Journal of Physical Chemistry Letters*, **2021**, 12, 9720-9729	6.4	4
77	Relief of excited-state antiaromaticity enables the smallest red emitter. *Nature Communications*, **2021**, 12, 5409	17.4	3
76	How Beneficial Is the Account of Doubly-Excited Configurations in Linear Response Theory?. *Journal of Chemical Theory and Computation*, **2021**, 17, 975-984	6.4	6
75	Computation of Molecular Ionization Energies Using an Ensemble Density Functional Theory Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 4489-4504	6.4	7
74	Next-generation quantum theory of atoms in molecules for the S1/S0 conical intersections in dynamics trajectories of a light-driven rotary molecular motor. *International Journal of Quantum Chemistry*, **2020**, 120, e26062	2.1	6
73	Mössbauer 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	3.6	4
72	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	3.6	3
71	Computation of Molecular Electron Affinities Using an Ensemble Density Functional Theory Method. *Journal of Physical Chemistry A*, **2020**, 124, 7795-7804	2.8	7

70	Performance Analysis and Optimization of Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) for Vertical Excitation Energies and Singlet-Triplet Energy Gaps. *Journal of Physical Chemistry A*, **2019**, 123, 7991-8000	2.8	17
69	Theoretical modelling of the dynamics of primary photoprocess of cyclopropanone. *Physical Chemistry Chemical Physics*, **2019**, 21, 2489-2498	3.6	17
68	Next-generation quantum theory of atoms in molecules for the photochemical ring-opening reactions of oxirane. *International Journal of Quantum Chemistry*, **2019**, 119, e25957	2.1	9
67	A 3-D bonding perspective of the factors influencing the relative stability of the S1/S0 conical intersections of the penta-2,4-dieniminium cation (PSB3). *International Journal of Quantum Chemistry*, **2019**, 119, e25903	2.1	7
66	Design and photoisomerization dynamics of a new family of synthetic 2-stroke light driven molecular rotary motors. *Chemical Communications*, **2019**, 55, 5247-5250	5.8	19
65	Formulation and Implementation of the Spin-Restricted Ensemble-Referenced Kohn-Sham Method in the Context of the Density Functional Tight Binding Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 3021-3032	6.4	5
64	Calculation of contact densities and Mössbauer 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	4
63	Conical Intersections in Organic Molecules: Benchmarking Mixed-Reference Spin-Flip Time-Dependent DFT (MRSF-TD-DFT) vs Spin-Flip TD-DFT. *Journal of Physical Chemistry A*, **2019**, 123, 6455-6462	2.8	20
62	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	26
61	Next-generation quantum theory of atoms in molecules for the ground and excited state of the ring-opening of cyclohexadiene. *International Journal of Quantum Chemistry*, **2019**, 119, e25862	2.1	13
60	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	6.4	27
59	Next-generation quantum theory of atoms in molecules for the ground and excited states of fulvene. *International Journal of Quantum Chemistry*, **2018**, 118, e25768	2.1	14
58	Fulgides as Light-Driven Molecular Rotary Motors: Computational Design of a Prototype Compound. *Journal of Physical Chemistry Letters*, **2018**, 9, 4995-5001	6.4	28
57	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	3.9	39
56	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
55	Description of ground and excited electronic states by ensemble density functional method with extended active space. *Journal of Chemical Physics*, **2017**, 147, 064104	3.9	23
54	Description of Conical Intersections with Density Functional Methods. *Topics in Current Chemistry*, **2016**, 368, 445-76		27
53	Ensemble DFT Approach to Excited States of Strongly Correlated Molecular Systems. *Topics in Current Chemistry*, **2016**, 368, 97-124		29

52	Design, Synthesis, and Dynamics of a Green Fluorescent Protein Fluorophore Mimic with an Ultrafast Switching Function. *Journal of the American Chemical Society*, **2016**, 138, 9807-25	16.4	32
51	Computational Design of a Family of Light-Driven Rotary Molecular Motors with Improved Quantum Efficiency. *Journal of Physical Chemistry Letters*, **2016**, 7, 105-10	6.4	48
50	Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. *Physical Chemistry Chemical Physics*, **2016**, 18, 21040-50	3.6	18
49	Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. *Journal of Chemical Physics*, **2016**, 145, 244104	3.9	21
48	A QTAIM and stress tensor investigation of the torsion path of a light-driven fluorene molecular rotary motor. *Journal of Computational Chemistry*, **2016**, 37, 2588-96	3.5	9
47	Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. *Journal of Chemical Physics*, **2015**, 142, 184104	3.9	31
46	Analytical energy gradient for the two-component normalized elimination of the small component method. *Journal of Chemical Physics*, **2015**, 142, 214106	3.9	24
45	Spin-restricted ensemble-referenced Kohn–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	7.9	88
44	Calculation of response properties with the normalized elimination of the small component method. *International Journal of Quantum Chemistry*, **2014**, 114, 993-1005	2.1	17
43	Assessment of approximate computational methods for conical intersections and branching plane vectors in organic molecules. *Journal of Chemical Physics*, **2014**, 141, 124122	3.9	56
42	Description of electron transfer in the ground and excited states of organic donor-acceptor systems by single-reference and multi-reference density functional methods. *Journal of Chemical Physics*, **2014**, 141, 124123	3.9	12
41	Dirac-exact relativistic methods: the normalized elimination of the small component method. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 436-467	7.9	35
40	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, 3074-84	6.4	132
39	Designing conical intersections for light-driven single molecule rotary motors: from precessional to axial motion. *Journal of Organic Chemistry*, **2014**, 79, 3587-600	4.2	53
38	Assessment of density functional theory based SCF (self-consistent field) and linear response methods for longest wavelength excited states of extended π-conjugated molecular systems. *Journal of Chemical Physics*, **2014**, 141, 024112	3.9	35
37	Understanding the dynamics behind photoisomerization of light-driven molecular rotary motors. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 427-437	7.9	8
36	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, 3917-32	6.4	78
35	Spin-orbit coupling calculations with the two-component normalized elimination of the small component method. *Journal of Chemical Physics*, **2013**, 139, 014106	3.9	36

34	Assessment of Density Functional Methods for Obtaining Geometries at Conical Intersections in Organic Molecules. *Journal of Chemical Theory and Computation*, **2013**, 9, 4526-4541	6.4	56
33	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, 2617-29	6.4	34
32	Analytic calculation of isotropic hyperfine structure constants using the normalized elimination of the small component formalism. *Journal of Physical Chemistry A*, **2012**, 116, 3481-6	2.8	31
31	Analytic Calculation of Contact Densities and Mössbauer Isomer Shifts Using the Normalized Elimination of the Small-Component Formalism. *Journal of Chemical Theory and Computation*, **2012**, 8, 875-82	6.4	33
30	Bondpseudorotation, Jahn-Teller, and pseudo-Jahn-Teller effects in the cyclopentadienyl cation and its pentahalogeno derivatives. *International Journal of Quantum Chemistry*, **2012**, 112, 3277-3288	2.1	17
29	Communication: On the isotope anomaly of nuclear quadrupole coupling in molecules. *Journal of Chemical Physics*, **2012**, 137, 131102	3.9	12
28	Relativistically corrected electric field gradients calculated with the normalized elimination of the small component formalism. *Journal of Chemical Physics*, **2012**, 137, 054113	3.9	19
27	An improved algorithm for the normalized elimination of the small-component method. *Theoretical Chemistry Accounts*, **2011**, 130, 633-644	1.9	36
26	On multiferroicity of TTF-CA molecular crystal. *Physical Chemistry Chemical Physics*, **2011**, 13, 144-8	3.6	13
25	Antiferromagnetic interactions in the quarter-filled organic conductor (EDO-TTF)2PF6. *Physical Chemistry Chemical Physics*, **2011**, 13, 12328-34	3.6	8
24	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, 2189-99	6.4	115
23	Understanding the dynamics behind the photoisomerization of a light-driven fluorene molecular rotary motor. *Journal of Physical Chemistry A*, **2010**, 114, 5058-67	2.8	83
22	Calibration of 57Fe isomer shift from ab initio calculations: can theory and experiment reach an agreement?. *Physical Chemistry Chemical Physics*, **2010**, 12, 2758-62	3.6	32
21	Calibration of 119Sn isomer shift using ab initio wave function methods. *Journal of Chemical Physics* , **2009**, 130, 124121	3.9	19
20	First principles calculation of Mössbauer isomer shift. *Coordination Chemistry Reviews*, **2009**, 253, 594-605	23.2	49
19	DFT Approach to the Calculation of Mössbauer Isomer Shifts. *Journal of Chemical Theory and Computation*, **2008**, 4, 278-85	6.4	36
18	Excitation energies from spin-restricted ensemble-referenced Kohn-Sham method: a state-average approach. *Journal of Physical Chemistry A*, **2008**, 112, 12980-8	2.8	49
17	Restricted Ensemble-Referenced Kohn-Sham versus Broken Symmetry Approaches in Density Functional Theory: Magnetic Coupling in Cu Binuclear Complexes. *Journal of Chemical Theory and Computation*, **2007**, 3, 764-74	6.4	102

16	On convergence of the normalized elimination of the small component (NESC) method. *Theoretical Chemistry Accounts*, **2007**, 117, 333-338	1.9	50
15	On the calculation of Mössbauer isomer shift. *Journal of Chemical Physics*, **2007**, 127, 084101	3.9	58
14	Comment on "Quasirelativistic theory equivalent to fully relativistic theory" [J. Chem. Phys. 123, 241102 (2005)]. *Journal of Chemical Physics*, **2006**, 125, 107101; discussion 107102	3.9	40
13	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	3.9	32
12	Implicit and Explicit Coverage of Multi-reference Effects by Density Functional Theory. *International Journal of Molecular Sciences*, **2002**, 3, 604-638	6.3	103
11	m-Benzyne and bicyclo[3.1.0]hexatriene – which isomer is more stable? – a quantum chemical investigation. *Chemical Physics Letters*, **2001**, 348, 115-125	2.5	61
10	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	2.3	30
9	Application of spin-restricted open-shell Kohn–Sham method to atomic and molecular multiplet states. *Journal of Chemical Physics*, **1999**, 110, 116-125	3.9	102
8	A spin-restricted ensemble-referenced Kohn–Sham method and its application to diradicaloid situations. *Chemical Physics Letters*, **1999**, 304, 429-437	2.5	183
7	Über den Neuanbindungs–Mechanismus der Alkanhydroxylierung durch Cytochrom P450: elektronische Struktur der Zwischenstufe und Charakter des Elektronentransfers bei der Neuanbindung. *Angewandte Chemie*, **1999**, 111, 3730-3733	3.6	11
6	On the "Rebound" 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	16.4	75
5	Tetramethyleneethane (TME) Diradical: Experiment and Density Functional Theory Reach an Agreement. *Journal of Physical Chemistry A*, **1999**, 103, 8885-8889	2.8	54
4	Spin-restricted density functional approach to the open-shell problem. *Chemical Physics Letters*, **1998**, 288, 689-697	2.5	124
3	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	4.8	303
2	Theoretical Investigation of Two-State-Reactivity Pathways of H–H Activation by FeO+: Addition–Elimination, Rebound, and Oxene-Insertion Mechanisms. *Journal of Physical Chemistry A* , **1998**, 102, 3835-3846	2.8	131
1	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm		2