

Michael Filatov

List of Publications by Citations

Source: <https://exaly.com/author-pdf/3133617/michael-filatov-publications-by-citations.pdf>

Version: 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm. <i>Chemistry - A European Journal</i> , 1998 , 4, 193-199	4.8	303
86	A spin-restricted ensemble-referenced Kohn-Sham method and its application to diradicaloid situations. <i>Chemical Physics Letters</i> , 1999 , 304, 429-437	2.5	183
85	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3074-84	6.4	132
84	Theoretical Investigation of Two-State-Reactivity Pathways of H ₂ Activation by FeO ⁺ : Addition-Elimination, Rebound, and Oxene-Insertion Mechanisms. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 3835-3846	2.8	131
83	Spin-restricted density functional approach to the open-shell problem. <i>Chemical Physics Letters</i> , 1998 , 288, 689-697	2.5	124
82	Surface Hopping Excited-State Dynamics Study of the Photoisomerization of a Light-Driven Fluorene Molecular Rotary Motor. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2189-99	6.4	115
81	Implicit and Explicit Coverage of Multi-reference Effects by Density Functional Theory. <i>International Journal of Molecular Sciences</i> , 2002 , 3, 604-638	6.3	103
80	Restricted Ensemble-Referenced Kohn-Sham versus Broken Symmetry Approaches in Density Functional Theory: Magnetic Coupling in Cu Binuclear Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 764-74	6.4	102
79	Application of spin-restricted open-shell Kohn-Sham method to atomic and molecular multiplet states. <i>Journal of Chemical Physics</i> , 1999 , 110, 116-125	3.9	102
78	Spin-restricted ensemble-referenced Kohn-Sham method: basic principles and application to strongly correlated ground and excited states of molecules. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2015 , 5, 146-167	7.9	88
77	Understanding the dynamics behind the photoisomerization of a light-driven fluorene molecular rotary motor. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 5058-67	2.8	83
76	Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3917-32	6.4	78
75	On the "Rebound" Mechanism of Alkane Hydroxylation by Cytochrome P450: Electronic Structure of the Intermediate and the Electron Transfer Character in the Rebound Step. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 3510-3512	16.4	75
74	m-Benzyne and bicyclo[3.1.0]hexatriene [which isomer is more stable?] a quantum chemical investigation. <i>Chemical Physics Letters</i> , 2001 , 348, 115-125	2.5	61
73	On the calculation of Mössbauer isomer shift. <i>Journal of Chemical Physics</i> , 2007 , 127, 084101	3.9	58
72	Assessment of approximate computational methods for conical intersections and branching plane vectors in organic molecules. <i>Journal of Chemical Physics</i> , 2014 , 141, 124122	3.9	56
71	Assessment of Density Functional Methods for Obtaining Geometries at Conical Intersections in Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4526-4541	6.4	56

70	Tetramethyleneethane (TME) Diradical: Experiment and Density Functional Theory Reach an Agreement. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 8885-8889	2.8	54
69	Designing conical intersections for light-driven single molecule rotary motors: from precessional to axial motion. <i>Journal of Organic Chemistry</i> , 2014 , 79, 3587-600	4.2	53
68	On convergence of the normalized elimination of the small component (NESC) method. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 333-338	1.9	50
67	First principles calculation of Mössbauer isomer shift. <i>Coordination Chemistry Reviews</i> , 2009 , 253, 594-605	23.2	49
66	Excitation energies from spin-restricted ensemble-referenced Kohn-Sham method: a state-average approach. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 12980-8	2.8	49
65	Computational Design of a Family of Light-Driven Rotary Molecular Motors with Improved Quantum Efficiency. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 105-10	6.4	48
64	Analytical derivatives of the individual state energies in ensemble density functional theory method. I. General formalism. <i>Journal of Chemical Physics</i> , 2017 , 147, 034113	3.9	42
63	Comment on "Quasirelativistic theory equivalent to fully relativistic theory" [J. Chem. Phys. 123, 241102 (2005)]. <i>Journal of Chemical Physics</i> , 2006 , 125, 107101; discussion 107102	3.9	40
62	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. <i>Journal of Chemical Physics</i> , 2018 , 149, 104101	3.9	39
61	Spin-orbit coupling calculations with the two-component normalized elimination of the small component method. <i>Journal of Chemical Physics</i> , 2013 , 139, 014106	3.9	36
60	An improved algorithm for the normalized elimination of the small-component method. <i>Theoretical Chemistry Accounts</i> , 2011 , 130, 633-644	1.9	36
59	DFT Approach to the Calculation of Mössbauer Isomer Shifts. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 278-85	6.4	36
58	Dirac-exact relativistic methods: the normalized elimination of the small component method. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014 , 4, 436-467	7.9	35
57	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. <i>Journal of Chemical Physics</i> , 2014 , 141, 024112	3.9	35
56	Development, Implementation, and Application of an Analytic Second Derivative Formalism for the Normalized Elimination of the Small Component Method. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2617-29	6.4	34
55	Analytic Calculation of Contact Densities and Mössbauer Isomer Shifts Using the Normalized Elimination of the Small-Component Formalism. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 875-82	6.4	33
54	Design, Synthesis, and Dynamics of a Green Fluorescent Protein Fluorophore Mimic with an Ultrafast Switching Function. <i>Journal of the American Chemical Society</i> , 2016 , 138, 9807-25	16.4	32
53	Calibration of ^{57}Fe isomer shift from ab initio calculations: can theory and experiment reach an agreement?. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 2758-62	3.6	32

52	Calculation of spin-densities within the context of density functional theory. The crucial role of the correlation functional. <i>Journal of Chemical Physics</i> , 2005 , 123, 124101	3.9	32
51	Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. <i>Journal of Chemical Physics</i> , 2015 , 142, 184104	3.9	31
50	Analytic calculation of isotropic hyperfine structure constants using the normalized elimination of the small component formalism. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3481-6	2.8	31
49	Alkane Hydroxylation by Cytochrome P450: Is Kinetic Isotope Effect a Reliable Probe of Transition State Structure?. <i>European Journal of Inorganic Chemistry</i> , 2000 , 2000, 2455-2458	2.3	30
48	Ensemble DFT Approach to Excited States of Strongly Correlated Molecular Systems. <i>Topics in Current Chemistry</i> , 2016 , 368, 97-124		29
47	Fulgides as Light-Driven Molecular Rotary Motors: Computational Design of a Prototype Compound. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4995-5001	6.4	28
46	Description of Conical Intersections with Density Functional Methods. <i>Topics in Current Chemistry</i> , 2016 , 368, 445-76		27
45	Direct Nonadiabatic Dynamics by Mixed Quantum-Classical Formalism Connected with Ensemble Density Functional Theory Method: Application to trans-Penta-2,4-dieniminium Cation. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4499-4512	6.4	27
44	Non-adiabatic dynamics of ring opening in cyclohexa-1,3-diene described by an ensemble density-functional theory method. <i>Molecular Physics</i> , 2019 , 117, 1128-1141	1.7	26
43	Analytical energy gradient for the two-component normalized elimination of the small component method. <i>Journal of Chemical Physics</i> , 2015 , 142, 214106	3.9	24
42	Description of ground and excited electronic states by ensemble density functional method with extended active space. <i>Journal of Chemical Physics</i> , 2017 , 147, 064104	3.9	23
41	Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. <i>Journal of Chemical Physics</i> , 2016 , 145, 244104	3.9	21
40	Conical Intersections in Organic Molecules: Benchmarking Mixed-Reference Spin-Flip Time-Dependent DFT (MRSF-TD-DFT) vs Spin-Flip TD-DFT. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6455-6462	2.8	20
39	Design and photoisomerization dynamics of a new family of synthetic 2-stroke light driven molecular rotary motors. <i>Chemical Communications</i> , 2019 , 55, 5247-5250	5.8	19
38	Calibration of ¹¹⁹ Sn isomer shift using ab initio wave function methods. <i>Journal of Chemical Physics</i> , 2009 , 130, 124121	3.9	19
37	Relativistically corrected electric field gradients calculated with the normalized elimination of the small component formalism. <i>Journal of Chemical Physics</i> , 2012 , 137, 054113	3.9	19
36	Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 21040-50	3.6	18
35	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. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 7991-8000	2.8	17

34	Theoretical modelling of the dynamics of primary photoprocess of cyclopropanone. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 2489-2498	3.6	17
33	Calculation of response properties with the normalized elimination of the small component method. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 993-1005	2.1	17
32	Bondpseudorotation, Jahn-Teller, and pseudo-Jahn-Teller effects in the cyclopentadienyl cation and its pentahalogeno derivatives. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 3277-3288	2.1	17
31	Next-generation quantum theory of atoms in molecules for the ground and excited states of fulvene. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25768	2.1	14
30	On multiferroicity of TTF-CA molecular crystal. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 144-8	3.6	13
29	Next-generation quantum theory of atoms in molecules for the ground and excited state of the ring-opening of cyclohexadiene. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25862	2.1	13
28	Description of electron transfer in the ground and excited states of organic donor-acceptor systems by single-reference and multi-reference density functional methods. <i>Journal of Chemical Physics</i> , 2014 , 141, 124123	3.9	12
27	Communication: On the isotope anomaly of nuclear quadrupole coupling in molecules. <i>Journal of Chemical Physics</i> , 2012 , 137, 131102	3.9	12
26	Über den Neuanbindungs-Mechanismus der Alkanhydroxylierung durch Cytochrom P450: elektronische Struktur der Zwischenstufe und Charakter des Elektronentransfers bei der Neuanbindung. <i>Angewandte Chemie</i> , 1999 , 111, 3730-3733	3.6	11
25	Next-generation quantum theory of atoms in molecules for the photochemical ring-opening reactions of oxirane. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25957	2.1	9
24	Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4339-4346	6.4	9
23	A QTAIM and stress tensor investigation of the torsion path of a light-driven fluorene molecular rotary motor. <i>Journal of Computational Chemistry</i> , 2016 , 37, 2588-96	3.5	9
22	Understanding the dynamics behind photoisomerization of light-driven molecular rotary motors. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013 , 3, 427-437	7.9	8
21	Antiferromagnetic interactions in the quarter-filled organic conductor (EDO-TTF)2PF6. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 12328-34	3.6	8
20	Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 848-859	6.4	8
19	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). <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25903	2.1	7
18	Computation of Molecular Ionization Energies Using an Ensemble Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4489-4504	6.4	7
17	Computation of Molecular Electron Affinities Using an Ensemble Density Functional Theory Method. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 7795-7804	2.8	7

16	Next-generation quantum theory of atoms in molecules for the S1/S0 conical intersections in dynamics trajectories of a light-driven rotary molecular motor. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26062	2.1	6
15	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). <i>Journal of Physical Chemistry A</i> , 2021 , 125, 1994-2006	2.8	6
14	Fast and Accurate Computation of Nonadiabatic Coupling Matrix Elements Using the Truncated Leibniz Formula and Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4722-4728	6.4	6
13	How Beneficial Is the Account of Doubly-Excited Configurations in Linear Response Theory?. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 975-984	6.4	6
12	Formulation and Implementation of the Spin-Restricted Ensemble-Referenced Kohn-Sham Method in the Context of the Density Functional Tight Binding Approach. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3021-3032	6.4	5
11	Calculation of contact densities and Mössbauer isomer shifts utilising the Dirac-exact two-component normalised elimination of the small component (2c-NESC) method. <i>Molecular Physics</i> , 2019 , 117, 1164-1171	1.7	4
10	Mössbauer isomer shifts and effective contact densities obtained by the exact two-component (X2C) relativistic method and its local variants. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 26776-26786	3.6	4
9	Analytical derivatives of the individual state energies in ensemble density functional theory. II. Implementation on graphical processing units (GPUs). <i>Journal of Chemical Physics</i> , 2021 , 154, 104108	3.9	4
8	Internal Conversion between Bright (1) and Dark (2) States in s-Butadiene and s-Hexatriene. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9720-9729	6.4	4
7	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. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 17567-17573	3.6	3
6	Relief of excited-state antiaromaticity enables the smallest red emitter. <i>Nature Communications</i> , 2021 , 12, 5409	17.4	3
5	Exploring Dyson's Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9963-9972	6.4	2
4	Description of Sudden Polarization in the Excited Electronic States with an Ensemble Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5123-5139	6.4	2
3	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm		2
2	Signatures of Conical Intersection Dynamics in the Time-Resolved Photoelectron Spectrum of Furan: Theoretical Modeling with an Ensemble Density Functional Theory Method. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	1
1	Manifestations of strong electron correlation in polyacene: Fundamental gap, density of states, and photoconductivity. <i>Carbon Trends</i> , 2022 , 7, 100146	0	0